

**EQUILIBRIUM PARTITIONING SEDIMENT
GUIDELINES (ESGs) FOR THE PROTECTION OF
BENTHIC ORGANISMS:
PAH MIXTURES**

**U. S. Environmental Protection Agency:
Office of Science and Technology and
Office of Research and Development**

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FOREWORD

Under the Clean Water Act (CWA), the U.S. Environmental Protection Agency (EPA) and the States develop programs for protecting the chemical, physical, and biological integrity of the nation's waters. To meet the objectives of the CWA, EPA has periodically issued ambient water quality criteria (WQC) beginning with the publication of "Water Quality Criteria, 1972" (NAS, 1973). The development of WQC is authorized by Section 304(a)(1), which directs the Administrator to develop and publish "criteria" reflecting the latest scientific knowledge on (1) kind and extent of effects on human health and welfare, including effects on plankton, fish, shellfish, and wildlife, that may be expected from the presence of pollutants in any body of water, including ground water; and (2) concentration and dispersal of pollutants on biological community diversity, productivity, and stability. All criteria guidance through late 1986 was summarized in an EPA document entitled "Quality Criteria for Water, 1986" (U.S. EPA, 1987). Updates on WQC documents for selected chemicals and new criteria recommendations for other pollutants have been more recently published as "National Recommended Water Quality Criteria-Correction" (U.S. EPA, 1999). The EPA will continue to update the nationally recommended WQC as needed in the future.

In addition to the development of WQC and to continue to meet the objectives of the CWA, EPA has conducted efforts to develop and publish equilibrium partitioning sediment guidelines (ESGs) for some of the 65 toxic pollutants or toxic pollutant categories. Toxic contaminants in bottom sediments of the nation's lakes, rivers, wetlands, and coastal waters create the potential for continued environmental degradation even where water column contaminant levels meet applicable water quality standards. In addition, contaminated sediments can lead to water quality impacts, even when direct discharges to the receiving water have ceased. These guidelines are authorized under Section 304(a)(2) of the CWA, which directs the Administrator to develop and publish information on, among other things, the factors necessary

1 to restore and maintain the chemical, physical, and biological integrity of all navigable waters.

2 The ESGs and associated methodology presented in this document are EPA's best recommendation
3 as to the concentrations of a substance that may be present in sediment while still protecting benthic
4 organisms from the effects of that substance. These guidelines are applicable to a variety of freshwater
5 and marine sediments because they are based on the biologically available concentration of the substance
6 in the sediments. These ESGs are intended to provide protection to benthic organisms from direct toxicity
7 due to this substance. In some cases, the additive toxicity for specific classes of toxicants (e.g., metal
8 mixtures or polycyclic aromatic hydrocarbon mixtures) is addressed. The ESGs do not protect against
9 synergistic or antagonistic effects of contaminants or bioaccumulative effects to benthos. They are not
10 protective of wildlife or human health endpoints.

11 EPA recommends that ESGs be used as a complement to existing sediment assessment tools, to help
12 assess the extent of sediment contamination, to help identify chemicals causing toxicity, and to serve as
13 targets for pollutant loading control measures. EPA is developing guidance to assist in the application of
14 these guidelines in water-related programs of the States and this Agency. This document provides guidance
15 to EPA Regions, States, the regulated community, and the public. It is designed to implement national
16 policy concerning the matters addressed. It does not, however, substitute for the CWA or EPA's
17 regulations, nor is it a regulation itself. Thus, it cannot impose legally binding requirements on EPA,
18 States, or the regulated community. EPA and State decision makers retain the discretion to adopt
19 approaches on a case-by-case basis that differ from this guidance where appropriate. EPA may change this
20 guidance in the future.

21 This document has been reviewed by EPA's Office of Science and Technology (Health and
22 Ecological Criteria Division, Washington, D.C.) and Office of Research and Development (Mid-Continent
23 Ecology Division, Duluth, MN; Atlantic Ecology Division, Narragansett, RI; Western Ecology Division,
24 Corvallis, OR), and approved for publication.

1 Mention of trade names or commercial products does not constitute endorsement or recommendation
2 of use.
3

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EXECUTIVE SUMMARY

This equilibrium partitioning sediment guideline (ESG) document recommends an approach for summing the toxicological contributions of mixtures of 34 PAHs in sediments to determine if their concentrations in any specific sediment would be protective of benthic organisms from their direct toxicity. The combination of the equilibrium partitioning (EqP), narcosis theory, and additivity provide the technical foundation for this guideline. These approaches were required because PAHs occur in sediments in a variety of proportions as mixtures and can be expected to act jointly under a common mode of action. Therefore, their combined toxicological contributions must be predicted on a sediment-specific basis. This overall approach provides for the derivation of an ESG that is causally linked to the specific mixtures of PAHs in a sediment, yet is applicable across sediments and appropriately protective of benthic organisms.

The EqP approach was chosen because it takes into account the varying biological availability of chemicals in different sediments and allows for incorporation of the appropriate biological effects concentration to predict the concentration of a nonionic organic chemical in sediment that is protective of benthic organisms. In its assertion, EqP theory holds that nonionic chemicals in sediment partition between sediment organic carbon, interstitial water and benthic organisms. At equilibrium, if the concentration in any one phase is known then the concentration in the others can be predicted. The ratio of the concentration in water to the concentration in organic carbon is termed the organic carbon partition coefficient (K_{OC}), which is a constant for each chemical. The ESG Technical Basis Document demonstrates that biological responses of benthic organisms to nonionic organic chemicals in sediments are different across sediments when the sediment concentrations are expressed on a dry weight basis, but similar when expressed on a μg chemical/g organic carbon (g_{OC}) basis. Responses were also similar across sediments when interstitial water concentrations were used to normalize biological

1 using the recommended uncertainty limits. The ESG for total PAH is the sum of the quotients of each
2 of the 34 individual PAHs in a specific sediment divided by the C_{OC,PAH_i,FCV_i} of that particular PAH.
3 This sum is termed the Equilibrium Partitioning Sediment Guideline Toxic Unit ($\Sigma ESGTU_{FCV}$) which is
4 based on the final chronic value. Sediments exhibiting $\leq 1.0 \Sigma ESGTU_{FCV}$ of the mixture of the 34
5 PAHs are acceptable for the protection of benthic organisms. This provides for the derivation of a
6 guideline that is causally linked to the specific mixtures of PAHs in a sediment, applicable across
7 sediments, and appropriately protective of benthic organisms.

8 This guideline does not protect against additive, synergistic or antagonistic effects of other
9 contaminants or bioaccumulative effects of PAHs to other aquatic life, wildlife or humans. Research is
10 needed to characterize the toxicological importance of PAHs not measured in this definition of total
11 PAH. It is the position of the Agency and the EPA Science Advisory Board (SAB) that the use of
12 equilibrium partitioning sediment guidelines as stand-alone, pass-fail criteria is not recommended for all
13 applications and should frequently trigger additional studies at sites under investigation. This ESG
14 applies only to sediments having $\geq 0.2\%$ organic carbon.

1 availability. The ESG Technical Basis Document further demonstrates that if the effect concentration
2 in water is known, the effect concentration in sediments on a $\mu\text{g}/\text{g}_{\text{OC}}$ basis can be accurately predicted
3 by multiplying the effect concentration in water by the chemical's K_{OC} . Because the water quality
4 criteria final chronic value (WQC FCV) is the concentration of a chemical in water that is protective of
5 the presence of aquatic life, and is appropriate for benthic organisms, the product of the WQC FCV
6 and K_{OC} is the concentration in sediments that on an organic carbon basis is protective of benthic
7 organisms.

8 Narcosis theory was used to (1) demonstrate that the slope of the acute toxicity- K_{OW}
9 relationship was similar across species; (2) normalize the acute toxicity of all PAHs in water to an
10 aquatic species to a reference K_{OW} of 1.0 (where the concentration in water and lipid of the organism
11 would be essentially the same); (3) establish an acute sensitivity ranking for individual species at the
12 K_{OW} of 1.0; and (4) to use the rankings and water-only acute-chronic ratios to calculate protective
13 concentrations of specific PAHs in tissues ($\mu\text{g}/\text{g}$ lipid) and water (FCV, $\mu\text{g}/\text{L}$) using the U.S. EPA
14 National Guidelines (Stephan et al., 1985). The EqP approach was then used to calculate the effect
15 concentration for these specific PAHs in sediment ($C_{\text{OC,PAH,FCV}}$, $\mu\text{g}/\text{g}$ organic carbon) from the product
16 of the PAH-specific FCV and K_{OC} .

17 Importantly, because PAHs occur in sediments as mixtures and their toxicities in water, tissues,
18 and sediments are additive or nearly additive, the consideration of their toxicities on an individual basis
19 would result in guidelines that are under-protective. For this reason the combined toxicological
20 contributions of the PAH mixture must be used. The U.S. EPA recommends the use of the 34 PAHs
21 monitored in the EMAP program to derive a concentration of "total PAH." Many monitoring and
22 assessment efforts measure a smaller group of PAHs, such as 13 or 23 PAHs; adjustment factors have
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7

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9 temperature.

GLOSSARY OF ABBREVIATIONS (continued)

1		
2	CV	Coefficient of Variation
3	CWA	Clean Water Act
4	DOC	Dissolved Organic Carbon
5	EC50	Concentration affecting 50% of the test organisms
6	EMAP	Environmental Monitoring and Assessment Program
7	EPA	United States Environmental Protection Agency
8	EqP	Equilibrium partitioning
9	ESG	Equilibrium Partitioning Sediment Guideline(s)
10	ESGTU _{FCV_i}	Equilibrium Partitioning Sediment Guideline Toxic Unit for PAH _i based on the FCV
11	ESGTU _{Rhepox}	Equilibrium Partitioning Sediment Guideline Toxic Unit for PAH _i based on the LC50
12		of <i>Rhepoxynius abronius</i> .
13	ΣESGTU _{FCV}	Sum of Equilibrium Partitioning Sediment Guideline Toxic Units, where the units are
14		based on FCV values
15	f_{Lipid}	Fraction of lipid in the organism
16	f_{OC}	Fraction of organic carbon in sediment
17	f_{SC}	Fraction of soot carbon in sediment
18	FACR	Final Acute-Chronic Ratio
19	FAV	Final Acute Value
20	FCV	Final Chronic Value
21	GMAV	Genus Mean Acute Value
22	IWTU	Interstitial Water Toxic Unit
23	IWTU _{FCV}	Interstitial water toxic unit calculated by dividing the dissolved interstitial water
24		concentration by the FCV

GLOSSARY OF ABBREVIATIONS

1		
2		
3	ACR	Acute-Chronic Ratio
4	AR	Approximate Randomization
5	ASTM	American Society for Testing and Materials
6	BaP	Benzo[a]pyrene
7	BCF	Bioconcentration factor
8	C_d	Freely-dissolved interstitial water concentration of contaminant
9	C_L	Chemical concentration in target lipid
10	C_L^*	Critical body burden in the lipid fraction of the organism
11	C_{OC}	Chemical concentration in sediments on an organic carbon basis
12	C_{OC,PAH_i}	PAH-specific chemical concentration in sediment on an organic carbon basis
13	$C_{octanol}$	Chemical concentration in octanol
14	C_{Org}	Chemical concentration in the organism
15	C_{Org}^*	Critical body burden in the organism
16	C_{IW}	Total interstitial water concentration of contaminant
17	$C_{OC,PAH_i,FCV}$	Effect concentration of a PAH in sediment on an organic carbon basis calculated from
18		the product of its FCV and K_{OC}
19	$C_{OC,PAH_i,Rhepox,LC50}$	Sediment LC50 concentration on an organic carbon basis for a specific PAH for
20		<i>Rhepoxinus</i> calculated from the product of its LC50 value at a K_{OW} of 1.0 and K_{OC}
21	$C_{OC,PAH_i,Max}$	Maximum solubility limited PAH concentration in sediment on an organic carbon basis
22		
23		
24		

GLOSSARY OF ABBREVIATIONS (continued)

1		
2	S	Aqueous Solubility
3	SAB	U.S. EPA Science Advisory Board
4	SE	Standard Error
5	SMAV	Species Mean Acute Value
6	SPARC	SPARC Performs Automated Reasoning in Chemistry
7	TOC	Total Organic Carbon
8	TU	Toxic Unit
9	WQC	Water Quality Criteria
10	WQCTU _{FCV}	Water Quality Criteria Toxic Unit based on the FCV

GLOSSARY OF ABBREVIATIONS (continued)

1		
2	K_{LW}	Lipid: water partition coefficient
3	K_{OC}	Organic carbon: water partition coefficient
4	K_{OW}	Octanol: water partition coefficient
5	K_p	Sediment: water partition coefficient
6	K_s	Setschenow constant
7	K_{SC}	Soot carbon: water partition coefficient
8	LC50	Concentration estimated to be lethal to 50 % of the test organisms within a specified
9		time period
10	LFER	Linear free energy relationship
11	MV	Molar Volume
12	NA	Not Applicable, Not Available
13	ND	Not Determined, Not Detected
14	NOAA	National Oceanographic and Atmospheric Administration
15	NOEC	No Observed Effect Concentration
16	NTU	Narcotic Toxic Units
17	OEC	Observable Effect Concentration
18	PAH	Polycyclic aromatic hydrocarbon
19	PAH _{OC}	Organic carbon-normalized PAH concentration in sediment
20	PCB	Polychlorinated Biphenyl
21	POC	Particulate Organic Carbon
22	PSTU	Predicted Sediment Toxic Units
23	QSAR	Quantitative Structure Activity Relationship
24	REMAP	Regional Environmental Monitoring and Assessment Program

1 contaminated sediments, to establish pollution prevention strategies, and to identify, prioritize and
2 implement appropriate clean up activities and source controls.

3 4 1.2 EQUILIBRIUM PARTITIONING AS A TECHNICAL BASIS FOR DERIVATION OF AN 5 ESG FOR MIXTURES OF PAHs 6

7 As a result of this need for technically defensible sediment guidelines to assist regulatory
8 agencies in making decisions concerning contaminated sediment problems and their prevention, a U.S.
9 EPA Office of Science and Technology and Office of Research and Development research team was
10 established to review alternative approaches (Chapman, 1987). All of the approaches reviewed had
11 both strengths and weaknesses and no single approach was found to be applicable for the derivation of
12 sediment guidelines in all situations (U.S. EPA, 1989a,b; U.S. EPA, 1992). The equilibrium
13 partitioning (EqP) approach was selected and first applied to nonionic organic chemicals because it
14 presented the greatest promise for generating defensible national numerical chemical specific guidelines
15 applicable across a broad range of sediment types (U.S. EPA, 2000a). Three principal observations
16 form the basis of the EqP method of deriving sediment guidelines for nonionic organic chemicals:

- 17 1. The concentration of nonionic organic chemicals in sediments, expressed on an organic
18 carbon basis, and in interstitial water correlate to observed biological effects on
19 sediment-dwelling organisms across a range of sediments.
20
- 21 2. Partitioning models can relate sediment concentrations for nonionic organic chemicals
22 on an organic carbon basis to freely-dissolved concentrations in interstitial water.
23
- 24 3. The distribution of sensitivities of benthic and water column organisms to chemicals are
25 similar; thus, the currently established WQC final chronic values (FCV) can be used to
26 define the acceptable effects concentration of a chemical freely-dissolved in interstitial
27 water.
28

SECTION 1

INTRODUCTION

1.1 LEGISLATIVE MANDATE AND NEED FOR ESGs

Under the Clean Water Act (CWA) the U.S. Environmental Protection Agency (EPA) is responsible for protecting the chemical, physical and biological integrity of the nation's waters. In keeping with this responsibility, U.S. EPA published ambient national water quality criteria (WQC) in 1980 for 64 of the 65 toxic pollutants or pollutant categories designated as toxic in the CWA. Additional water quality documents that update criteria for selected consent decree chemicals and new criteria have been published since 1980. These national WQC are numerical concentration limits that are the U.S. EPA's best estimate of the concentrations in water that are protective of human health and of aquatic life. While these WQC play an important role in assuring a healthy aquatic environment, they alone are not sufficient to ensure the protection of environmental or human health.

Toxic pollutants in bottom sediments of the nation's lakes, rivers, wetlands, estuaries and marine coastal waters pose many ecological and human health risks throughout the United States (U.S. EPA, 1997a,b,c). Contaminated sediments create the potential for continued environmental degradation even where water column concentrations comply with established human health and aquatic life WQC. In addition, contaminated sediments can be a significant pollutant source that may cause water quality degradation to persist, even when other pollutant sources are controlled (Larsson, 1985; Salomons et al., 1987; Burgess and Scott, 1992; U.S. EPA, 1997a,b,c). The development of defensible numerical chemical specific concentration limits of substances applicable across a range of sediment types (sediment guidelines) is needed to accurately assess the extent of the ecological risks of

1 Over the past 15 years, the U. S. EPA research team and others have been working together to
2 investigate the toxicity and bioavailability of sediment contaminants to benthic organisms. As a result
3 of this effort, the Agency has developed the "Technical Basis for the Derivation of Equilibrium
4 Partitioning Sediment Guidelines (ESGs) for the Protection of Benthic Organisms: Nonionic Organics
5 (U.S. EPA, 2000a). In addition, U. S. EPA has developed a document describing the further use of
6 the EqP method for deriving ESGs for mixtures of the metals cadmium, copper, lead, nickel, silver
7 and zinc (U.S. EPA, 2000b). This methodology has been reviewed both by the U.S. EPA Science
8 Advisory Board and through the public comment process. The Agency also has developed ESGs for
9 the pesticides dieldrin and endrin (U.S. EPA, 2000c,d) and proposed ESGs for the individual
10 polycyclic aromatic hydrocarbons (PAHs) acenaphthene, fluoranthene and phenanthrene (U.S. EPA
11 1993a,b,c). Because PAHs occur in the environment as mixtures, rather than single chemicals, ESGs
12 for individual PAHs have the potential to be substantially under-protective because they do not account
13 for other co-occurring PAHs. The ESGs for individual PAHs have therefore been withdrawn.

14 Numerous efforts have previously sought to address and estimate the toxicity of PAH mixtures
15 (PTI Environmental Services, 1991; Long et al., 1995). However, the resultant sediment guidelines
16 have engendered considerable controversy over such issues as the correlative versus causal relations
17 between dry weight sediment chemistry and biological effects, the bioavailability of sediment
18 contaminants, the effects of covarying chemicals and mixtures, and ecological relevance (Swartz et al.,
19 1999). The U. S. EPA research team has concluded, based upon additional investigation, that issuance
20 of sediment guidelines for PAHs based on EqP was necessary to resolve these outstanding issues. Most
21 importantly, the ESGs must be based on mixtures of PAHs to be adequately protective of benthic
22 organisms, as well as ecologically relevant.

23 The EPAH model developed by Swartz et al. (1995) and based upon a combination of the EqP
24 approach, quantitative structure activity relationships (QSAR), narcosis theory, and concentration

1 addition models provided initial insight into a technical approach for resolving these complexities. This
2 EqP-based ΣPAH model provides a method to address causality, account for bioavailability, consider
3 mixtures, and predict toxicity and ecological effects. The most significant contribution to the
4 development of the scientific basis for deriving ESGs for PAH mixtures is described by Di Toro et al.
5 (2000) and Di Toro and McGrath (2000). This pioneering research forms major portions of this
6 document.

7 8 1.3 OVERVIEW OF THIS DOCUMENT

9
10 This document presents the theoretical basis and supporting data relevant to the derivation of
11 ESGs for mixtures of PAHs.

12 Section 2 of this document "Narcosis Theory: Model Development and Application for PAH
13 Mixtures" contains an analysis of the narcosis and EqP models to demonstrate the scientific basis for
14 the derivation of WQC and ESGs for mixtures of narcotic chemicals, including PAHs. Data are
15 presented that demonstrate that the toxicity of narcotic chemicals increase with K_{ow} and that the slope
16 of the K_{ow} -toxicity relationship is not different across species. The universal slope of this relationship
17 (-0.945) is applicable for all narcotic chemical classes, whereas the intercept is chemical class-specific.
18 The intercept of this slope at a K_{ow} of 1.0 predicts the tissue effect concentration. The toxicities of
19 mixtures of narcotic chemicals in water are shown to be approximately additive, thus the toxic unit
20 concept is applicable to mixtures. The toxicities of narcotic chemicals are shown to be limited by their
21 solubilities in water, hence their toxicities in sediments are limited.

22 Section 3 of this document "Toxicity of PAHs in Water and Derivation of National PAH-
23 specific FCVs" presents an analysis of acute and chronic water-only toxicity data for freshwater and
24 saltwater aquatic organisms exposed to individual PAHs. It examines (1) the relative sensitivities of

1 freshwater and saltwater organisms to determine if separate FCVs are required, and (2) the relative
2 sensitivities of benthic organisms and organisms used to derive WQC to determine if the WQC FCV
3 should be based only on benthic organisms. These data are used with the narcosis model presented in
4 Section 2, the EqP approach (U.S. EPA, 2000a), and the U.S. EPA National WQC Guidelines
5 (Stephan et al., 1985) to derive the WQC FCV for individual PAHs (PAH-specific FCV).

6 Section 4 "Derivation of ESG" contains the approach used for deriving the ESGs for mixtures
7 of PAHs. The C_{OC,PAH_i,FCV_i} is derived for each individual PAH as the product of the PAH-specific FCV
8 and the respective K_{OC} value as recommended by the EqP approach. The use of the C_{OC,PAH_i,FCV_i} value
9 for individual PAHs is inappropriate for use as the ESG because PAHs occur as mixtures. The
10 toxicities of mixtures of narcotic chemicals have been shown to be approximately additive, therefore,
11 combined toxic contributions of all PAHs in the mixture can be determined by summing the quotients
12 of the concentration of each PAH in the sediment divided by its C_{OC,PAH_i,FCV_i} to determine the sum of
13 these Equilibrium Partitioning Sediment Guideline Toxic Units ($\Sigma ESGTU_{FCV}$). If the $\Sigma ESGTU_{FCV}$ is
14 ≤ 1.0 , the sediment guideline for the PAH mixture is not exceeded and the PAH concentration in the
15 sediment is protective of benthic organisms. If the $\Sigma ESGTU_{FCV}$ exceeds 1.0, the sediment guideline for
16 the PAH mixture is exceeded and sensitive benthic organisms may be affected by the PAHs. The ESG
17 derived for PAH mixtures is compared to concentrations of PAH mixtures in sediments from national
18 monitoring programs to reveal the incidence of sediment guideline exceedences. An example
19 calculation is provided to explain the conversion of concentrations of individual PAHs on a dry weight
20 basis into the guideline.

21 Section 5 "Toxicity of PAHs: PAHs in Spiked and Field Sediments" examines the applicability
22 of the EqP methodology for C_{OC,PAH_i,FCV_i} and ESG derivation. The C_{OC,PAH_i,FCV_i} and ESG are compared
23 to (1) databases of observed sediment toxicity and benthic community impacts in sediments spiked with
24 PAHs, and (2) sediments from the field where PAHs are the probable contaminants of concern.

1 Section 6 "Implementation" defines the PAHs to which the ESG apply and examines the photo-
2 activation of PAHs in UV sunlight and teratogenicity and carcinogenicity of certain PAHs in the
3 mixture. The importance of equilibrium and the partitioning of PAHs to other organic carbon phases
4 (e.g. soot and coal) is described. An approach for calculating PAH solubilities for temperatures or
5 salinities at a specific site is provided. The implementation of the PAH mixture ESG by various U. S.
6 EPA Program Offices using different regulatory mandates is addressed separately in the
7 "Implementation Framework for Use of Equilibrium Partitioning Sediment Guidelines" (U.S. EPA,
8 2000e).

9 Section 7 "Sediment Guideline Statement" presents the sediment guideline statement
10 recommended by U. S. EPA. Concerns that the user will need to be aware of are listed.

11 Section 8 "References" lists references cited in all sections of this document.

SECTION 2

NARCOSIS THEORY: MODEL DEVELOPMENT AND APPLICATION FOR PAH MIXTURES

2.1 SECTION OVERVIEW

This section of the ESG document presents a model of the toxicity of narcotic chemicals to aquatic organisms that is applicable to the derivation of WQC and ESGs for mixtures of narcotic chemicals, including PAHs. Both the model and this section of the document are largely excerpted from the pioneering publications of Di Toro et al. (2000) and Di Toro and McGrath (2000) which should be consulted for components of the overall model that are not included in this ESG document. The narcosis model includes a scientific analysis of the toxicities of narcotic chemicals fundamental to the derivation of WQC and ESGs for their mixtures. The ESG for PAH mixtures described in Section 4 of this document is derived using this model and toxicity data exclusively for PAHs (see Section 3).

The narcosis model is used to describe the toxicity of all type I narcotic chemicals. Since PAHs are expected to be type I narcotic chemicals (Hermens, 1989; Verhaar et al., 1992), the toxicological principles that apply to them should be more accurately characterized by an analysis of the principles that apply to narcotic chemicals overall. Model development utilizes a database of LC50 values comprising 156 chemicals and 33 species, including fish, amphibians, arthropods, molluscs, annelids, coelenterates and echinoderms. The analysis detailed in this section is used to demonstrate that (1) the toxicities of narcotic chemicals, and therefore PAHs, are dependant on the chemical's K_{ow} ; (2) the slope of the K_{ow} -toxicity relationship is the same for all species of aquatic organisms and classes of narcotic chemicals with the intercepts being species and chemical class-specific; (3) the species-specific LC50 values normalized to a $K_{ow} = 1.0$ permit ranking of species sensitivities and are

equivalent to the body burden LC50 on a lipid basis; and (4) the toxicities of mixtures of narcotic chemicals are additive.

The analysis of narcotic chemical toxicity data presented in this section shows that the proposed model accounts for the variations in toxicity due to differing species sensitivities and chemical differences. The model is based on the idea that the target lipid is the site of action in the organism. Further, it is assumed that target lipid has the same lipid-octanol linear free energy relationship for all species. This implies that the $\log_{10}\text{LC50}$ vs $\log_{10}K_{\text{ow}}$ slope is the same for all species. However, individual species may have varying target lipid body burdens of narcotic chemicals that cause mortality. The target lipid LC50 body burdens estimated by extrapolations from the water-only acute toxicity data and K_{ow} values are compared to measured total lipid LC50 body burdens for five species. They are essentially equal, indicating that the extrapolation in the model is appropriate for estimation of LC50 body burdens, i.e., that the target lipid concentration is equal to the total extracted lipid concentration. The precise relationship between target lipid and octanol is established.

2.2 NARCOSIS MODEL BACKGROUND

A comprehensive model of type I narcosis chemicals that considers multiple species has been presented by Van Leeuwen et al. (1992). They developed QSARs for individual species and performed species sensitivity analysis. A similar analysis is presented in Di Toro et al. (2000). The key differences in the Di Toro et al. (2000) model are the use of a single universal slope for the $\log_{10}\text{LC50}$ versus $\log_{10}K_{\text{ow}}$ QSAR for all the species, the inclusion of corrections for chemical classes, such as PAHs, that are slightly more potent than baseline narcotics, and the interpretation of the y-intercepts as the species-specific critical body burdens for narcosis mortality.

2.3 BODY BURDEN MODEL

The initial quantitative structure-activity models for narcotic toxicity relied on correlations of $\log_{10}LC50$ and $\log_{10}K_{ow}$ (Konemann, 1981; Veith et al., 1983). An interesting and important interpretation of this inverse relationship that relates the toxicity to chemical body burden has been presented by McCarty et al. (1991), and proceeds as follows. The relationship between the LC50 (mmol/L) and K_{ow} for fish is approximately

$$\log_{10}LC50 \approx -\log_{10}K_{ow} + 1.7 \quad (2-1)$$

For each LC50, a fish body burden on a wet weight basis corresponding to narcosis mortality can be computed using a bioconcentration factor BCF (L/kg) which is defined as the ratio of the chemical concentration in the organism C_{org} (mmol/kg) to the chemical concentration dissolved in the water C_d (mmol/L)

$$BCF = \frac{C_{org}}{C_d} \quad (2-2)$$

Using the BCF the organism concentration corresponding to the LC50, which is referred to as the critical body burden and denoted by C_{org}^* , can be computed using

$$C_{org}^* = BCF \times LC50 \quad (2-3)$$

The superscript * indicates that it is a critical body burden corresponding to the LC50. The BCF also

varies with K_{OW} . For fish, the relationship is

$$\log_{10} BCF \approx \log_{10} K_{OW} - 1.3 \quad (2-4)$$

Therefore, the critical body burden corresponding to the LC50 for fish narcosis can be computed using the narcosis LC50 and the BCF

$$\log_{10} C_{Org}^* = \log_{10} BCF + \log_{10} LC50$$

$$\approx \log_{10} K_{OW} - 1.3 - \log_{10} K_{OW} + 1.7$$

$$\approx 0.4 \quad (2-5)$$

or

$$C_{Org}^* \approx 2.5 \mu\text{mol/g wet wt} \quad (2-6)$$

Thus, McCarty et al. (1991) rationalize the relationship between LC50 values and K_{OW} by suggesting that mortality is caused as a result of a constant body burden of the narcotic chemical.

The reason the critical body burden is a constant concentration for all the narcotic chemicals represented by the narcosis LC50 is a consequence of the unity slopes for $\log_{10} K_{OW}$ in Equations 2-1 and 2-4. If the fraction of lipid in the fish is assumed to be 5% ($f_{Lipid} = 0.05$), then the critical body burden in the lipid fraction of the fish is

$$C_L^* = \frac{C_{Org}^*}{f_{Lipid}} \approx 50 \mu\text{mol/g lipid} \quad (2-7)$$

1 which is the estimate of the chemical concentration in the lipid of these fish that causes 50% mortality.
2 The model presented below is an extension of this idea.

3 4 2.4 TARGET LIPID MODEL

5
6 The body burden model relates the narcosis concentration to a whole body concentration using
7 a BCF. If different species are tested, then species-specific BCFs would be required to convert the
8 LC50 concentration to a body burden for each species. A more direct approach is to relate narcotic
9 lethality to the concentration of the chemical in the target tissue of the organism, rather than to the
10 concentration in the whole organism. If the partitioning into the target tissue is independent of species,
11 then the need for species-specific BCFs is obviated. The identity of the target tissue is still being
12 debated (Abernethy et al., 1988; Franks and Lieb, 1990), but we assume that the target is a lipid
13 fraction of the organism. Hence the name, target lipid.

14 The target lipid model is based on the assumption that mortality occurs when the chemical
15 concentration in the target lipid reaches a threshold concentration. This threshold is assumed to be
16 species-specific rather than a universal constant that is applicable to all organisms (e.g., 50 $\mu\text{mol/g}$
17 lipid, see Equation 2-7). The formulation follows the body burden model (McCarty et al., 1991). The
18 target lipid-water partition coefficient K_{LW} (L/kg lipid) is defined as the ratio of chemical concentration
19 in target lipid, C_L ($\mu\text{mol/g lipid} = \text{mmol/kg lipid}$), to the freely-dissolved aqueous concentration C_d ,
20 (mmol/L)

$$22 \quad K_{LW} = \frac{C_L}{C_d} \quad (2-8)$$

This equation can be used to compute the chemical concentration in the target lipid phase producing narcotic mortality, i.e., the critical body burden in the lipid fraction C_L^* , when the chemical concentration in the water phase is equal to the LC50

$$C_L^* = K_{LW} \times LC50 \quad (2-9)$$

Assuming the narcosis hypothesis is true, i.e., that 50 % mortality occurs if *any* narcotic chemical reaches the concentration C_L^* , then the LC50 for any chemical can be calculated using the same critical target lipid concentration C_L^* and the chemical-specific target lipid-water partition coefficient

$$LC50 = \frac{C_L^*}{K_{LW}} \quad (2-10)$$

or

$$\log_{10} LC50 = \log_{10} C_L^* - \log_{10} K_{LW} \quad (2-11)$$

The problem is determining the K_{LW} for narcotic chemicals. It is commonly observed for classes of organic molecules that the logarithms of the partition coefficient between two liquids are related by a straight line (Leo, 1972). For target lipid and octanol, the relationship would be

$$\log_{10} K_{LW} = a_0 + a_1 \log_{10} K_{OW} \quad (2-12)$$

Such a relationship is called a linear free energy relationship (LFER) (Brezonik, 1994). Combining

Equations 2-11 and 2-12 yields the following linear relationship between $\log_{10}LC50$ and $\log_{10}K_{ow}$

$$\log_{10}LC50 = \log_{10}C_L^* - a_0 - a_1 \log_{10}K_{ow} \quad (2-13)$$

where $\log_{10}C_L^* - a_0$ is the y intercept and $-a_1$ is the slope of the line.

This derivation produces the linear relationship between $\log_{10}LC50$ and $\log_{10}K_{ow}$ which is found experimentally (see, for example, Table 4 in Hermens et al., 1984)

$$\log_{10}LC50 = m \log_{10}K_{ow} + b \quad (2-14)$$

where m and b are the slope and intercept of the regression, respectively. In addition, it identifies the meanings of the parameters of the regression line. The slope of the line m is the negative of the slope of the LFER between target lipid and octanol, a_1 . The intercept of the regression $b = \log_{10}C_L^* - a_0$ is composed of two parameters: C_L^* is the target lipid concentration at narcosis mortality, and a_0 is the constant in Equation 2-12.

The difference between the target lipid model and the McCarty et al. (1991) body burden model is that for the latter, the coefficients a_0 and a_1 for fish are assumed to be known: $a_0 = -1.3$ and $a_1 = 1.0$. It is interesting to examine the consequences of a similar assumption applied to the target lipid model. If it is assumed that the partitioning of narcotic chemicals in lipid and octanol are equal, i.e., that lipid is octanol, a common first approximation, then $a_1 = 1$ and $a_0 = 0$ and the y-intercept becomes

$$b = \log_{10}C_L^* \quad (2-15)$$

which is the target-lipid concentration producing 50% narcosis mortality.

This result can be understood by examining Figure 2-1. The y-intercept b is the LC50 value for a chemical with a $\log_{10}K_{OW} = 0$ or $K_{OW} = 1$. The K_{OW} is the ratio of the chemical's concentration in octanol to its concentration in water. Hence, for this hypothetical chemical (an example would be 2-chloroethanol for which $\log_{10}K_{OW} = -0.048 \approx 0$) the chemical's concentration in water is equal to its concentration in octanol. However, if the K_{LW} equals the K_{OW} , i.e., lipid is octanol, then its concentration in water must be equal to its concentration in the target lipid of the organism. Therefore, the y-intercept is the target lipid phase concentration at which 50% mortality is observed. That is

$$LC50|_{K_{OW}=1} = b = C_{Octanol} = C_L^* \quad (2-16)$$

Note that this interpretation is true only if $a_0 = 0$ (see Equation 2-13).

Thus the target lipid narcosis model differentiates between the chemical and biological parameters of the $\log_{10}LC50 - \log_{10}K_{OW}$ regression coefficients in the following way

Regression Coefficients		Chemical	Biological
Slope:	$m =$	$-a_1$	
Intercept:	$b =$	$-a_0$	$+ \log_{10}C_L^*$

(2-17)

The chemical parameters a_0 and a_1 are associated with the LFER between octanol and target lipid (Equation 2-12). The biological parameter is the critical target lipid concentration C_L^* . This result is important because it suggests that the slope $m = -a_1$ of the $\log_{10}LC50 - \log_{10}K_{OW}$ relationship should be the *same* regardless of the species tested since it is a chemical property of the target lipid - the slope of the LFER. Of course this assumes that the target lipid of all species have the same LFER relative to

1 octanol. This seems to be a reasonable expectation since the mechanism of narcosis is presumed to
2 involve the phospholipids in the cell membrane and it appears to be a ubiquitous mode of action.
3 However, the biological component of the intercept C_L^* (Equations 2-13 and 2-17) should vary with
4 species sensitivity to narcosis since it is commonly found that different species have varying sensitivity
5 to the effects of exposure to the same chemical. The expectations that follow from the target lipid
6 model - that the slope should be constant among species and that the intercepts should vary among
7 species - is the basis for the data analysis presented below.

8 9 2.5 ACUTE LETHALITY DATABASE COMPILATION

10
11 An acute lethality (LC50) database for type I narcotics from water-only toxicity tests was
12 compiled from available literature sources. The principal criterion for acceptance was that a number of
13 chemicals were tested using the same species so that the slope and intercept of the $\log_{10}LC50 - \log_{10}K_{ow}$
14 relationship could be estimated. The data were restricted to acute exposures and a mortality end point
15 to limit the sources of variability. A total of 33 species including amphibians, fishes, arthropods
16 (insects and crustaceans), molluscs, annelids, coelenterates and protozoans were represented. Seventy-
17 four individual datasets were selected for inclusion in the database which provided a total of 796
18 individual data points. Details are provided in Appendix A. The individual chemicals which comprise
19 the database are listed in Appendix B. There are 156 different chemicals including halogenated and
20 non-halogenated aliphatic and aromatic hydrocarbons, PAHs, alcohols, ethers, furans, and ketones.

21 The $\log_{10}K_{ow}$ values and aqueous solubilities of these chemicals were determined using SPARC
22 (SPARC Performs Automated Reasoning in Chemistry) (Karickhoff et al., 1991), which utilizes the
23 chemical's structure to estimate various properties. The reliability of SPARC was tested using $\log_{10}K_{ow}$
24 values measured using the slow stir flask technique (de Bruijn et al., 1989). Fifty three compounds

1 such as phenols, anilines, chlorinated monobenzenes, PAHs, PCBs and pesticides were employed. A
2 comparison of the $\log_{10}K_{OW}$ values measured using the slow stir flask technique to the SPARC estimates
3 demonstrates that SPARC can be used to reliably estimate measured $\log_{10}K_{OW}$ values over nearly a
4 seven order of magnitude range of $\log_{10}K_{OW}$ (Figure 2-2A). Note that this comparison tests both
5 SPARC and the slow stir measurements, since SPARC is not parameterized using octanol-water
6 partition coefficients (Hilal et al., 1994).

7 8 2.5.1 Aqueous Solubility

9
10 The toxicity data were screened by comparing the LC50 value to the aqueous solubility, S , of
11 the chemical (Figure 2-2B). (Note: For this and other figures in this document where a large number
12 of data points are available, the plotting procedure limits the actual number of data plotted.) Individual
13 LC50 values were eliminated from the database if the $LC50 > S$, which indicated the presence of a
14 separate chemical phase in the experiment. For these cases, mortality must have occurred for reasons
15 other than narcosis – for example the effect of the pure liquid on respiratory surfaces – since the target
16 lipid concentration cannot increase above that achieved at the water solubility concentration. A total of
17 55 data points were eliminated, decreasing the number to 736 and the number of individual chemicals
18 to 145 (Appendix B).

19 20 2.5.2 Exposure Duration

21
22 The duration of exposure varies in the dataset from 24 to 96 hours (Appendix A). Before the
23 data can be combined for analysis, the individual datasets need to be adjusted to account for this
24 difference. The required equilibration time may vary with both organism and chemical. An increase

1 in either organism body size or chemical hydrophobicity may increase the time to reach equilibrium.

2 To determine if acute lethality for narcotic chemicals varied with exposure time, data were
3 selected where toxicity was reported at multiple exposure times for the same organism and the same
4 chemical. For seven fish species, data were available for 96 hours and either 24, 48 or both 24 and 48
5 hours exposure. Arithmetic ratios of the LC50 values for 48 and 96 hours and for the 24 and 96 hours
6 exposures are compared to $\log_{10}K_{OW}$. The 48 to 96 hour ratio is 1.0 for essentially all the data (Figure
7 2-3A). The 24 to 96 hour ratio is larger, approaching 2.0 for the higher K_{OW} chemicals (Figure 2-3B).
8 A linear regression is used to fit the relationship in Figure 2-3B.

9

$$10 \quad LC50_{(24)}/LC50_{(96)} = 0.0988 \log_{10}K_{OW} + 0.9807 \quad (2-18)$$

11

12 where $LC50_{(24)}$ and $LC50_{(96)}$ are the LC50 values for 24 and 96 hour exposures. Since the majority of
13 the data points, approximately 46%, in the overall database represent narcosis mortality after exposure
14 to a chemical for 96 hours, the 24-hour fish toxicity data are converted to a 96 hour LC50 value using
15 Equation 2-18 for chemicals having $\log_{10}K_{OW}$ values where the ratio is > 1 . No correction factor is
16 applied to 24 hour toxicity data for invertebrates and fishes exposed to chemicals having $\log_{10}K_{OW}$
17 values where the ratio is < 1 (Di Toro et al., 2000).

18

19 2.6 DATA ANALYSIS

20

21 The analysis of the toxicity data is based on the target lipid model assumption that the slope of
22 the $\log_{10}LC50 - \log_{10}K_{OW}$ is the same for all species. This assumption was tested using a linear
23 regression model to estimate the species-specific body burdens and the universal narcosis slope.

2.6.1 Regression Model

Consider a species k and a chemical j . The $LC50_{k,j}$ for that species-chemical pair is

$$\log_{10}LC50_{k,j} = \log_{10}C_L^*(k) - a_0 - a_1 \log_{10}K_{ow}(j) \quad (2-19)$$

$$= b_k - a_1 \log_{10}K_{ow}(j) \quad (2-20)$$

where

$$b_k = \log_{10}C_L^*(k) - a_0 \quad (2-21)$$

is the y-intercept. The problem to be solved is: how to include all the b_k , $k = 1, \dots, N_s$ corresponding to the $N_s = 33$ species and a single slope a_1 in one multiple linear regression model equation.

The solution is to use a set of indicator variables δ_{ki} that are either zero or one depending on the species associated with the observation being considered. The definition is

$$\delta_{ki} = 1 \quad k = i \quad (2-22)$$

$$\delta_{ki} = 0 \quad k \neq i$$

which is the Kronecker delta (Kreyszig, 1972). The regression equation can be formulated using δ_{ki} as follows

$$\log_{10}LC50_{i,j} = a_1 \log_{10}K_{ow}(j) + \sum_{k=1}^{N_s} b_k \delta_{ki} \quad (2-23)$$

Equation 2-23 is now a linear equation with $N_s + 1$ independent variables: $\log_{10}K_{ow}(j)$ and δ_{ki} , $k = 1, \dots, N_s$. There are $N_s + 1$ coefficients to be fit: a_1 and b_k , $k = 1, \dots, N_s$. For each $LC50_{ij}$ corresponding to species i and chemical j , one of the b_k corresponding to the appropriate species $k = i$ has a unity coefficient $\delta_{ii} = 1$ while the others are zero. The way to visualize this situation is to realize that each row of data consists of the $LC50$ and these $N_s + 1$ independent variables, for example for $j = 1$ and $i = 3$

$\log_{10}LC50_{ij}$	$\log_{10}K_{ow}(j)$	δ_{1i}	δ_{2i}	δ_{3i}	...	$\delta_{N_s i}$
0.788	1.175	0	0	1	0	0

(2-24)

which is actually the first of the 736 records in the database. The result is that b_3 is entered into the regression equation as the intercept term associated with species $i = 3$ because that δ_{ki} is one for that record. By contrast, the slope term $a_1 \log_{10}K_{ow}(j)$ is always included in the regression because there is always an entry in the $\log_{10}K_{ow}(j)$ column (Equation 2-24). Hence the multiple linear regression estimates the common slope a_1 and the species-specific intercepts b_k , $k = 1, \dots, N_s$.

A graphical comparison of the results of fitting Equation 2-23 to the full dataset are shown in Figure 2-4 for each of the 33 species. The regression coefficients are tabulated and discussed subsequently after a further refinement is made to the model. The lines appear to be representative of the data as a whole. There appear to be no significant deviations from the common slope. A few outliers, which are plotted as +, were not included in the regression analysis. An outlier is identified if the difference between predicted and observed $LC50$ value is greater than one log unit when they are included in the regression. This decreases the total number of data points from 736 to 722.

2.6.2 Testing The Model Assumptions

The adequacy of the regression model is tested by answering three questions:

1. Are the data consistent with the assumption that the slope is the same for each species tested?
2. Does the volume fraction hypothesis (Abernethy et al., 1988) provide a better fit?
3. Are there systematic variations for particular chemical classes?

The first assumption, that the slope estimated for a particular species is statistically indistinguishable from the universal slope $a_1 = -0.97$ without chemical class correction (see Section 2.6.4), can be tested using conventional statistical tests for linear regression analysis (Wilkinson, 1990). The method is to fit the data for each species individually to determine a species-specific slope. Then, that slope is tested against the universal slope $a_1 = -0.97$ without chemical class correction to determine the probability that this difference could have occurred by chance alone. The probability and the number of data points for each species are shown in Figure 2-5A. The slope deviations are shown in Figure 2-5B. Some of the slope deviations are quite large. However, only three species equal or exceed the conventional significance level of 5% for rejecting the equal slope hypothesis.

Testing at the 5% level of significance is misleading, however, because there is more than an even chance of rejecting one species falsely when 33 species are being tested simultaneously. The reason is that the expected number of rejections for a 5% level of significance would be $33 \times 0.05 = 1.65$, i.e., more than one species on average would be rejected due to statistical fluctuations even though all the slopes are actually equal. In fact, only 20 tests at 5% would, on average, yield one slope that would be incorrectly judged as different. The correct level of significance is $(1/33)(1/20) = 0.152\%$ so that the expected number of rejections is $33 \times 0.00152 = 0.05$ or 5% (Wilkinson, 1990). This level of significance is displayed together with the slope data presented in Figure 2-5A. As can be

seen, there is no statistical evidence for rejecting the claim of equal slopes for the tested species. As would be expected, when 5% was used as the level of significance two species were identified as having unique slopes. When the current level of significance (0.00152) was used for the 33 samples none were different.

2.6.3 Volume Fraction Hypothesis

The volume fraction hypothesis asserts that narcotic mortality occurs at a constant volume fraction of chemical at the target site of the organism (Abernethy et al., 1988). Basically, this involves expressing the LC50 as a volume fraction of chemical rather than a molar concentration. This is done using the molar volume of the chemicals (see column MV in Appendix B). The LC50 on a molar volume basis is

$$LC50(\text{cm}^3/\text{L}) = LC50(\text{mmol/L}) \times MV(\text{cm}^3/\text{mmol}) \quad (2-25)$$

The question is: does using molar volume as the concentration unit improve the regression analysis?

The results are shown below

LC50	mmol/L	cm ³ /L
Slope	-0.97 ± 0.012	-0.90 ± 0.012
R ²	0.94	0.96

The R² value for the volume fraction analysis (0.96) is slightly greater than that for concentrations based on more standard units of concentration (0.94). Because they are essentially the same this document uses the standard units of concentration rather than those based on the volume fraction.

1 Importantly, the slope for both volume and weight units of concentration is not unity.

2 3 2.6.4 Chemical Classes 4

5 The analysis presented above assumes that all the 145 chemicals listed in Appendix B are
6 narcotic chemicals. That is, the only distinguishing chemical property that affects their toxicity is K_{ow} .
7 A criteria has been suggested that can be used to determine whether a chemical is a narcotic (Bradbury
8 et al., 1989), namely that it demonstrates additive toxicity with a reference narcotic. However, it is not
9 practical to test each possible chemical. The more practical test is whether the toxicity can be predicted
10 solely from the $\log_{10}LC50 - \log_{10}K_{ow}$ regression. In fact, this is used in methods that attempt to
11 discriminate baseline narcotics from other classes of organic chemicals (Verhaar et al., 1992).

12 Using this approach, differences in toxicity among chemical classes would be difficult to detect
13 if differing species were aggregated or different slopes were allowed in the regression analysis.
14 However, with the large dataset employed above, these differences can be seen by analyzing the
15 residuals grouped by chemical class.

16 The criteria for choosing the relevant classes are not obvious without a detailed understanding
17 of the mechanism of narcotic toxicity. Hence, the conventional organic chemical classes based on
18 structural similarities, e.g. ethers, alcohols, ketones, etc., are used. The results are shown in Figure 2-
19 6A. The means ± 2 standard error (SE) of the means are shown for each class. Although not a
20 rigorous test, the ± 2 SE range does not encompass zero for certain classes. Thus, it is likely that there
21 are statistically significant chemical class effects.

22 23 2.6.4.1 Statistical Analysis of K_{ow} -Toxicity Relationships 24

A rigorous test is conducted by including correction constants for each of the chemical classes in a manner that is analogous to Equation 2-23. The model equation is formulated using $N_C - 1$ corrections, Δc_ℓ , corresponding to the $\ell = 1, \dots, N_C - 1$ chemical classes. These are interpreted as corrections relative to the baseline class that is chosen to be aliphatic non-halogenated hydrocarbons. The regression equation is formulated as before with a variable $\xi_{\ell j}$ that is one if chemical j is in chemical class ℓ and zero otherwise

$$\begin{aligned}\xi_{\ell j} &= 1 && \text{if chemical } j \text{ is in class } \ell \\ \xi_{\ell j} &= 0 && \text{otherwise}\end{aligned}\tag{2-26}$$

The regression equation that results is

$$\log_{10} \text{LC50}_{i,j} = a_1 \log_{10} K_{\text{OW}}(j) + \sum_{k=1}^{N_S} b_k \delta_{ki} + \sum_{\ell=1}^{N_C-1} \Delta c_\ell \xi_{\ell j}\tag{2-27}$$

Each data record now contains the dependent variable $\log_{10} \text{LC50}_{i,j}$, the independent variables $\log_{10} K_{\text{OW}}$, $\log_{10} K_{\text{OW}}(j)$, and the δ_{ki} , $k = 1, \dots, N_S$ and $\xi_{\ell j}$, $\ell = 1, \dots, N_C - 1$ indicator variables which are 0 or 1 depending on which species and which chemical class is represented by the $\text{LC50}_{i,j}$.

Only $N_C - 1$ chemical class corrections are required because including N_C class corrections under-determines the equation set with one too many unknowns. The reason is that every equation would have one b_i and one Δc_ℓ for species i and chemical j in chemical class ℓ . Since this condition would occur in every equation there is no unique solution for the b_k and the Δc_ℓ values. One of these constants could be adjusted by an arbitrary amount and the rest could then be adjusted to compensate while still achieving the same fit of the data. Thus, a reference chemical class is chosen: non-halogenated aliphatic hydrocarbons for which $\Delta c_\ell = 0$. The remaining regression constants Δc_ℓ , $\ell =$

1 1,...,Nc - 1 are then the differential toxicity of chemical class ℓ relative to the reference class. This is
2 the reason for the Δc notation.

3 The requirement for a chemical class correction is decided using a statistical test that compares
4 the Δc_ℓ values that result from the regression to the hypothesis $\Delta c_\ell = 0$. For the classes which are not
5 statistically different, they are included in the baseline class and the parameters are re-estimated. This
6 is continued until all the remaining Δc_ℓ values are statistically different from zero. After a number of
7 trials, it was found that treating halogen substitutions as a separate additive correction gave the least
8 number of statistically significant class corrections. Thus chemical class corrections are applied to the
9 base structure if necessary and an additional correction is made if any substitute is a halogen. Thus for
10 halogenated chemicals it is possible that two $\xi_g = 1$ in Equation 2-27. The chemical classes are listed
11 in Appendix B.

12 The results of the final regression analysis are listed in Table 2-1. Both the logarithmic b_i and
13 arithmetic 10^{b_i} values of the intercepts are included together with their standard errors. Chemical
14 classes that demonstrate higher potency than the reference class are ketones and PAHs. Halogenation
15 increases the potency as well. After accounting for different potencies in the chemical classes, the
16 mean residuals are statistically indistinguishable from zero (Figure 2-6B).

17 18 2.6.4.2 Standard Errors And Residuals

19
20 The standard errors of the body burdens $SE(b_i)$ found from the regression (Equation 2-27) are
21 in an almost one-to-one correspondence with the number of data points for that species. Thus the b_i for
22 *Pimephales* with 182 data points has a 10% coefficient of variation, $CV(b_i) = SE(b_i) / b_i$, while the b_i
23 for *Neanthes* with 4 data points has a 50% coefficient of variation (Table 2-1). The relationship of the
24 sample size (N) to the coefficient of variation of the estimated critical body burden, $CV(b_i)$, is shown in

Figure 2-7A.

The residuals are log normally distributed (Figure 2-7B) and exhibit no trend with respect to K_{ow} (Figure 2-7C) which confirms the assumption underlying the use of regression analysis. The reason they are restricted to ± 1 order of magnitude is that 14 data points outside that range were originally excluded as outliers (for some values previously less than \pm one order of magnitude, chemical class corrections produced values slightly greater than one order of magnitude as shown in Figure 2-7C).

2.6.4.3 Chemical Class Corrections

The corrections due to chemical classes reduce the critical body burden by a factor of approximately one-half for ketones and PAHs. Halogenation reduces it further by 0.570 (Table 2-1). Thus a chlorinated PAH would exhibit a critical body burden of approximately one-third of a baseline narcotic. The coefficients of variation for these corrections are approximately 10%.

The chemical class differences among the type I narcotics affect the $LC50-K_{ow}$ relationship. The model no longer predicts a single straight line for the $\log_{10}LC50-\log_{10}K_{ow}$ relationship for all narcotic chemicals. What is happening is that the y-intercepts are changing due to the changing Δc_i values. The model (Equation 2-27) when applied to a single species k is

$$\log_{10}LC50_{kj} = a_1 \log_{10}K_{ow}(j) + b_k + \sum_{i=1}^{N_C-1} \Delta c_i \xi_{ij} \quad (2-28)$$

This is a straight line if only baseline narcotics are considered $\Delta c_i = 0$ or if only one chemical class correction is involved, e.g., all halogenated baseline narcotics. Otherwise more than one Δc_i enter into

Equation 2-28 and the line is jagged. Figure 2-8 presents three examples. The deviations from the baseline narcosis straight line are caused by the different chemical class potencies.

2.7 UNIVERSAL NARCOSIS SLOPE

The universal narcosis slope: $m = -0.945 \pm 0.014$ that results from the final analysis that includes chemical class corrections (Table 2-1) is smaller than that determined above without chemical class corrections (-0.97 ± 0.012). It is close to unity, a value commonly found (Hansch and Leo, 1995), and larger than the average of individual slopes (-0.86 ± 0.14) reported by Van Leeuwen et al. (1992), but comparable with a recent estimate for fathead minnows of -0.94 (Russom et al., 1997).

The fact that the slope is not exactly one suggests that octanol is not quite lipid. However, it is also possible that for the more hydrophobic chemicals in the database, the exposure time may not have been long enough for complete equilibration of water and lipid to have occurred. To test this hypothesis, the regression analysis is restricted to successively smaller upper limits of $\log_{10}K_{ow}$. The results are listed below

Maximum $\log_{10}K_{ow}$	3.5	4.0	4.5	5.0	5.5
Slope	-0.959	-0.970	-0.958	-0.950	-0.945
Standard Error	0.018	0.015	0.015	0.014	0.015

The variation is within the standard errors of estimation, indicating that there is no statistically significant difference if the higher $\log_{10}K_{ow}$ data are removed from the regression. This suggests that the universal narcosis slope is not minus one but is actually -0.945 ± 0.014 .

One consequence of the use of a universal narcosis slope is that the species sensitivity ranking derived from comparing either the water-only LC50 values or the critical body burdens of various

species are the same. This occurs because the critical body burden is calculated from the LC50 value and the universal slope (Equations 2-14 and 2-15)

$$\log_{10}C_L^* = \log_{10}LC50 + 0.945\log_{10}K_{ow} \quad (2-29)$$

If this were not the case, then the species sensitivity order could be reversed if LC50 values or C_L^* were considered.

Equation 2-29 is important because it can be used to compute the critical body burden of any type I narcotic chemical. Thus it predicts what the critical body burden should be for a particular species at its LC50 value. This would be the concentration that would be compared to a directly measured critical body burden. It can be thought of as a normalization procedure that corrects type I narcotics for the varying K_{ow} and places them on a common footing, namely, the critical body burden.

The motivation for the development of the target lipid model was to apply it to mixtures of PAHs and other persistent narcotic chemicals in sediments. The narcosis database used to determine the universal narcosis slope and the critical body burdens consists of 145 chemicals, of which 10 are un-substituted and substituted PAHs (Di Toro and McGrath, 2000). A comparison of the LC50 data for just these chemicals and the target lipid model is shown in Figure 2-9. The solid $\log_{10}LC50 - \log_{10}K_{ow}$ lines are computed using the universal narcosis slope and the appropriate body burdens for PAHs for each organism listed. The dotted lines apply to the chloronaphthalenes which have a slightly lower critical body burden due to the halogen substitution. The lines are an adequate fit of the data, although the scatter in the *Daphnia* data is larger than some of the other species with multiple sources of data and there is a clear outlier for *Americamysis*. It is for this reason that the slope representing all data for narcosis chemicals is used to derive the target lipid concentration from water-only toxicity data for PAHs in Section 3 of this document.

2.8 COMPARISON TO OBSERVED BODY BURDENS

The target lipid model predicts the concentration in octanol (the y-intercept) that causes 50% mortality in 96 hours. The question is: how do these compare to measured critical body burdens? The species-specific y-intercepts, b_i , are related to the target lipid concentration by the relationship

$$\text{y-intercept} = b_i = \log_{10} C_L^*(i) - a_0 \quad (2-30)$$

or, with chemical class corrections,

$$\text{y-intercept} = b_i + \Delta c_\ell = \log_{10} C_L^*(i) - a_0 \quad (2-31)$$

for species i and chemical class ℓ , where a_0 is the parameter in the LFER between octanol and target lipid (Equation 2-12).

The relationship between the predicted concentration in octanol, $b_i + \Delta c_\ell$, to the concentration measured in extracted lipid, $\log_{10} C_L^*$, is examined in Table 2-2 which lists observed LC50 body burdens ($\mu\text{mol/g}$ lipid) and predicted critical body burdens ($\mu\text{mol/g}$ octanol) for organisms in the database for which measured lipid-normalized critical body burdens were available. Three fish species: *Gambusia affinis* (mosquito fish), *Poecilia reitculata* (guppy) and *Pimephales promelas* (fathead minnow), and two crustaceans: *Leptocheirus plumulosus* (amphipod) and *Portunus pelagicus* (crab) are compared in Figure 2-10. The predicted and measured body burdens differ by less than a factor of 1.6. The fish were observed to have higher critical body burdens than the crustaceans, which the model reproduces.

The apparent near equality between the estimated and measured critical body burdens, which come from two independent sets of data, strongly suggest that in fact

$$a_0 = 0 \quad (2-32)$$

so that

$$\log_{10} C_L(i) = b_i + \Delta c_i = \text{y-intercept} \quad (2-33)$$

This relationship implies that the target lipid is the lipid measured by the extraction technique used in the body burden datasets. This is an important practical result since it suggests that body burdens normalized to extracted lipid are expressed relative to the appropriate phase for narcotic toxicity. Since the intercepts appear to be the organism's lipid concentration, the y-intercepts ($b_i + \Delta c_i$) in the discussion presented below are referred to as body burden lipid concentrations although the units ($\mu\text{mol/g}$ octanol) are retained since these are, in fact, the actual units of the intercepts.

2.9 MIXTURES AND ADDITIVITY

Narcotic chemicals, including PAHs, occur in the environment as mixtures, therefore, their mixture effects need to be appropriately resolved. If the toxicity of mixtures is additive, mixture effects can be assessed using the concept of toxic units. A toxic unit TU is defined as the ratio of the concentration in a medium to the effect concentration in that medium.

The additivity of the toxicity of narcotic chemicals in water has been demonstrated by a number of investigators. The results of mixture experiments which employed a large enough number of narcotic chemicals so that non-additive behavior would be detected is presented in Figure 2-11 as adopted from Hermens (1989). Three of the four experiments demonstrated essentially additive behavior and the fourth, a chronic exposure, was almost additive.

2.10 AQUEOUS SOLUBILITY CONSTRAINT

The existence of the need for a solubility cutoff for toxicity was suggested by Veith et al. (1983) based on data from fathead minnows (*P. promelas*) and guppies (*P. reticulata*). The highest dissolved concentration in water that can be achieved by a chemical is its aqueous solubility, S . Therefore, the maximum lipid concentration that can be achieved is limited as well. It is for this reason that the LC50 database is limited to chemicals with $\log_{10}K_{ow} \leq 5.3$. This is also the reason that the LC50 database that was used to generate the FCVs for specific PAHs in Section 3 of this document, was screened initially for LC50 values $\leq S$, using the solubilities from Mackay et al. (1992), rather than $\log_{10}K_{ow} \leq 5.3$ used by Di Toro et al. (2000).

For sediments, a solubility constraint should be applied as well. This is readily calculated using the relationship between interstitial water and the organic carbon-normalized sediment concentration. Since the interstitial water concentration is limited by S , the sediment concentration should be limited by the concentration in sediment organic carbon that is in equilibrium with the interstitial water at the aqueous solubility. Therefore, observed sediment concentrations are limited by the condition

$$C_{oc} \leq C_{oc,max} = K_{oc}S \quad (2-34)$$

SECTION 3

TOXICITY OF PAHs IN WATER AND DERIVATION OF PAH-SPECIFIC FCVs

3.1 NARCOSIS THEORY, EqP THEORY AND WQC GUIDELINES: DERIVATION OF PAH-SPECIFIC FCVs FOR INDIVIDUAL PAHs

Polycyclic aromatic hydrocarbons occur in the environment as mixtures. Therefore, in order to adequately protect aquatic life the approach used to derive a WQC FCV or sediment guideline for PAHs must account for their interactions as a mixture. In this section we present an approach for deriving FCVs for individual PAHs which can be used to derive the ESG for mixtures of PAHs.

Concepts developed by Di Toro et al. (2000) and presented in Section 2 of this document provide the technical framework for screening and analyzing aquatic toxicity data on PAHs. In particular, Section 2 demonstrated that: (1) the universal slope of the K_{ow} -toxicity relationship for narcotic chemicals is the same for all aquatic species; and (2) the intercept of the slope at a K_{ow} of 1.0 for each species provides the LC50/EC50 in $\mu\text{mol/g}$ octanol that indicates the critical body burden in and relative sensitivities of each species.

These concepts permit the use of the U.S. EPA National WQC Guidelines (Stephan et al., 1985) to derive WQC FCVs for individual PAHs and PAH mixtures. The universal slope is used with PAH-specific LC50/EC50 values to derive test-specific K_{ow} normalized reference acute values at a K_{ow} of 1.0. (This is analogous to the hardness normalization used to derive WQC for metals). These values are used to calculate species mean acute values (SMAVs) and genus mean acute values (GMAVs): (1) because only acute and chronic toxicity data from water-only tests with freshwater and saltwater species exposed to individual PAHs are used, a PAH chemical class correction is not needed; (2) the data are screened for acceptability following the requirements for use of species resident to

1 North America, test durations, test quality, etc. of the U.S. EPA National WQC Guidelines (Stephan et
2 al., 1985); (3) the individual acute values are adjusted using the universal slope of the K_{ow} -toxicity
3 relationship from the narcotic chemical analysis that was shown to apply to all aquatic species in
4 Section 2 to derive the acute value at a K_{ow} of 1.0 (Appendix C); (4) the intercept of the slope at a K_{ow}
5 of 1.0 for each species provides the LC50/EC50 in $\mu\text{mol/g}$ octanol that indicates the relative sensitivity
6 of each species, which was used to calculate SMAVs and GMAVs in $\mu\text{mol/g}$ octanol, which are
7 indicative of critical tissue concentrations in organisms on a $\mu\text{mol/g}$ lipid basis. The GMAVs are used
8 to calculate the final acute value (FAV) applicable to PAHs at a K_{ow} of 1.0 (Stephan et al., 1985).
9 This FAV at a K_{ow} of 1.0, when divided by the Final Acute-Chronic Ratio (FACR), becomes the FCV
10 at a K_{ow} of 1.0. Importantly, the FCV for any specific PAH can then be derived by back calculating
11 using its specific K_{ow} and the universal narcosis slope. When the PAH-specific FCV exceeds the
12 known solubility of that PAH, the maximum contribution of that PAH to the toxicity of the mixture is
13 set at the K_{oc} multiplied by the solubility of that PAH.

14 The FCV for PAH mixtures derived in this section of the document differs slightly from that
15 which would be derived for other narcotic chemicals in that it: (1) is derived using only acute and
16 chronic toxicity data from water-only tests with freshwater and saltwater species exposed to individual
17 PAHs, therefore, the data do not require the PAH chemical class correction; (2) the data are rigorously
18 screened for acceptability following the requirements for the use of species resident to North America,
19 test durations, test quality, etc. of the U.S. EPA National WQC Guidelines (Stephan et al., 1985). The
20 last search of the literature on the toxicity of PAHs was completed in January 2000.

3.2 ACUTE TOXICITY OF INDIVIDUAL PAHS: WATER EXPOSURES

3.2.1 Acute Toxicity of PAHs

One hundred and four acute water-only toxicity tests with 12 different PAHs have been conducted on 24 freshwater species from 20 genera that meet the requirements of the U.S. EPA National WQC Guidelines (Stephan et al. 1985, see Appendix C). The tested life-stages of 15 of the genera were benthic (infaunal or epibenthic). The most commonly tested freshwater species were the cladocerans (*Daphnia magna*) and (*Daphnia pulex*), rainbow trout (*Oncorhynchus mykiss*), fathead minnow (*P. promelas*) and bluegill (*Lepomis macrochirus*). The most commonly tested PAHs with freshwater organisms were acenaphthene, fluoranthene, fluorene, naphthalene, phenanthrene and pyrene.

Seventy-seven acute water-only toxicity tests with 8 different PAHs have been conducted on 30 saltwater species from 29 genera (Appendix C). The tested life-stages of 21 of the genera were benthic (infaunal or epibenthic). The most commonly tested saltwater species were the annelid worm (*Neanthes arenaceodentata*), mysid (*Americamysis bahia*), grass shrimp (*Palaemonetes pugio*), pink salmon (*Oncorhynchus gorbuscha*), and sheepshead minnow (*Cyprinodon variegatus*). The most commonly tested PAHs with saltwater organisms were acenaphthene, fluoranthene, naphthalene, phenanthrene and pyrene.

3.2.2 Acute Values at a K_{ow} of 1.0

The LC50 values or EC50 values where the effect is likely lethal, ($\mu\text{g/L}$) from individual acute toxicity tests from Appendix C were used to derive the GMAV ($\mu\text{mol/g}$ octanol) at a K_{ow} of 1.0. The

1 goal of this process was to convert individual LC50 or EC50 values that vary for a species across
2 PAHs into PAH-specific GMAVs at a K_{ow} of 1.0. The use of normalizing factors in WQC derivation
3 is not unique to this document. It is analogous to the hardness adjustment applied to the freshwater
4 WQC for cadmium, copper, lead, nickel and zinc and the pH and temperature adjustments applied to
5 the freshwater WQC for ammonia. For multiple PAHs tested against one species, the K_{ow}
6 normalization should result in similar PAH-specific SMAVs. Initially, the LC50 or EC50 values in
7 $\mu\text{g/L}$ were compared to the known solubility in water of the PAH tested. If the published LC50 or
8 EC50 concentration exceeded the solubility of the tested PAH, the concentration of the PAH at
9 solubility is listed in bold in Appendix C as a "greater than" acute value to indicate that the actual
10 toxicity of the dissolved PAH was unknown, though likely greater than solubility. For these tests, this
11 greater than solubility value, and not the published LC50 or EC50 value which is enclosed in
12 parentheses in Appendix C, was used in further calculations only when there were no acute values for
13 that species at concentrations less than the solubility. Next, the LC50, EC50 or greater than solubility
14 value was converted to μmol of the tested PAH/L. When the same PAH was tested more than once
15 against a species, the geometric mean of all LC50 or EC50 values was calculated to determine the
16 PAH-specific SMAV. The -0.945 universal slope of the toxicity/ K_{ow} relationship (Equation 2-29) was
17 applied to the PAH-Specific SMAVs ($\mu\text{mol/L}$) to calculate the PAH-specific SMAV ($\mu\text{mol/g}$ octanol)
18 at a $K_{ow}=1.0$. This should result in similar PAH-specific SMAVs for each of the PAHs tested. The
19 SMAV for all tested PAHs is the geometric mean of the PAH-Specific SMAVs at a K_{ow} of 1.0. The
20 GMAV ($\mu\text{mol/g}$ octanol) at a K_{ow} of 1.0 is the geometric mean of the SMAVs at a K_{ow} of 1.0.

21 The SMAVs at a K_{ow} of 1.0 were similar for multiple PAHs (Appendix C). For 21 freshwater
22 and saltwater species, two to nine different PAHs were tested. The range in ratios of the highest to
23 lowest acute values for multiple PAHs tested against an individual species before normalization was
24 1.98 to 186; an average ratio of 43.2. In contrast, the range in the ratios of the highest to lowest PAH-

specific SMAVs at a K_{ow} of 1.0 was 1.14 to 12.2; average ratio of 4.80. For 10 of the 21 (56%) species tested against multiple PAHs, the ratio of high to low SMAVs at a K_{ow} of 1.0 was 4.0 or less. This compares favorably with the factor of four or less difference in the acute values for 12 of 19 (63%) of the same species in multiple tests with the same PAH. Therefore, the variability of SMAVs at a K_{ow} of 1.0 across PAHs is similar to the variability inherent in acute toxicity testing with only one PAH. This suggests that the GMAVs provide data across PAHs that indicate the relative sensitivity of that species that can be used to describe species at risk and to calculate the FAV.

The acute sensitivities of freshwater and saltwater genera and the sensitivities of benthic and benthic plus water column genera do not differ (see Section 3.4). Therefore, GMAVs at a K_{ow} of 1.0 can be used to indicate the relative sensitivities for all freshwater and saltwater genera (Figure 3-1). The K_{ow} -normalized GMAVs (not including values greater than the solubility of the tested PAH) range from 7.66 $\mu\text{mol/g}$ octanol for *Americamysis* to 187 $\mu\text{mol/g}$ octanol for *Tanytarsus*, a factor of only 24.4. Saltwater genera constitute four of the five genera with GMAVs at a K_{ow} of 1.0 within a factor of two of the most sensitive genus (*Americamysis*). Of the 49 genera, the most sensitive one-third include a freshwater hydra, two amphipods, an insect, saltwater fish, a crab, two mysids, two shrimp, and three saltwater amphipods. All of these 16 genera have GMAVs at a K_{ow} of 1.0 that are within a factor of three, and 14 of the genera are benthic. Benthic and water column genera are distributed throughout the sensitivity distributions indicating that they have similar sensitivities. Genera that are benthic have been tested more frequently than water column genera.

3.3 CHRONIC TOXICITY OF INDIVIDUAL PAHS: WATER EXPOSURES

3.3.1 Acenaphthene

1 Chronic life-cycle toxicity tests have been conducted with acenaphthene with the freshwater
2 midge (*Paratanytarsus* sp.) and the saltwater mysid (*A. bahia*), and early life-stage tests have been
3 conducted with the fathead minnow (*P. promelas*) and sheepshead minnow (*C. variegatus*) (Table 3-1).
4 For each of these species, one or more benthic life-stages were exposed. Other chronic toxicity tests
5 have been conducted with the freshwater chironomid (*Paratanytarsus* sp.) and *P. promelas* (Lemke et
6 al., 1983; Lemke, 1984; Lemke and Anderson, 1984) but insufficient documentation is available to
7 permit use of these results (Thursby, 1991a).

8 Two acceptable life-cycle toxicity tests have been conducted with *Paratanytarsus* sp.
9 (Northwestern Aquatic Sciences, 1982). In the first test, 575 $\mu\text{g/L}$ reduced survival 90%, reduced
10 growth 60%, and all eggs failed to hatch (Table 3-1). No adverse effects occurred at acenaphthene
11 concentrations up to 295 $\mu\text{g/L}$ acenaphthene. In the second test, survival was reduced 20% and growth
12 30% at 315 $\mu\text{g/L}$. Egg hatchability was not affected in the highest concentration of 676 $\mu\text{g/L}$; although
13 survival of hatched larvae was reduced ~60%. No significant effects were observed at acenaphthene
14 concentrations up to 164 $\mu\text{g/L}$.

15 A total of six early life-stage toxicity tests have been conducted with the *P. promelas* as part of
16 a round-robin test series; two each from three laboratories (Table 3-1) (Academy of Natural Sciences,
17 1981; ERCO, 1981; Cairns and Nebeker, 1982). The lowest observed effect concentrations (LOEC)
18 across laboratories and tests ranged from 98 to 509 $\mu\text{g/L}$, a factor of 5.2. Growth (dry weight),
19 survival, or both growth and survival were reduced. Only one of these test pairs had a suitable
20 measured acute value that allowed calculation of an acute-chronic ratio, or ACR (Cairns and Nebeker,
21 1982). The concentration-response relationships were similar for the two tests of Cairns and Nebeker
22 (1982). In the first test, the early life-stages of this fish were unaffected in acenaphthene concentrations
23 ranging from 67 to 332 $\mu\text{g/L}$, but 495 $\mu\text{g/L}$ reduced growth 54% relative to control fish. In the second
24 test, growth was reduced 30% at 509 $\mu\text{g/L}$, but no effects were detected in fish exposed to 197 to 345

1 $\mu\text{g/L}$.

2 Data from saltwater chronic toxicity tests with acenaphthene are available for *A. bahia* and *C.*
3 *variegatus*. Reproduction of *A. bahia* was affected by acenaphthene in two life-cycle tests from two
4 different laboratories. In the first test (Horne et al., 1983), 340 $\mu\text{g/L}$ reduced reproduction 93 %
5 relative to controls and all *A. bahia* died at 510 $\mu\text{g/L}$. No effects were observed on the parental
6 generation at 100 to 240 $\mu\text{g/L}$ and second generation juveniles were not affected at $\leq 340 \mu\text{g/L}$. In the
7 second test (Thursby et al., 1989b), no effects were observed at $\leq 44.6 \mu\text{g/L}$, but a concentration of
8 91.8 $\mu\text{g/L}$ reduced reproduction 91 %. No reproduction occurred at higher concentrations, and growth
9 was reduced 34 % at 168 $\mu\text{g/L}$ and survival 96 % at 354 $\mu\text{g/L}$.

10 A test with early life-stages of *C. variegatus* showed that 240 to 520 $\mu\text{g/L}$ had no effects, but
11 that concentrations of 970, 2,000 and 2,800 $\mu\text{g/L}$, respectively, reduced survival of embryos and
12 larvae by $\geq 70\%$ (Table 3-1; Ward et al., 1981).

13 In general, the above results show that the difference between acute and chronic toxicity of
14 acenaphthene is small and differed minimally between species (Table 3-2). Species mean acute-chronic
15 ratios for acenaphthene are 6.68 for *Paratanytarsus sp.*, 1.48 for *P. promelas*, 3.42 for *A. bahia* and
16 4.36 for *C. variegatus*.

17 18 3.3.2 Anthracene

19
20 A single life-cycle toxicity test has been conducted with *D. magna* exposed to only three
21 concentrations of anthracene (Holst and Geisey, 1989). Minimal decreases were observed on the
22 number of broods produced in all three of the concentrations tested: 2.1 $\mu\text{g/L}$ (5.3 %), 4.0 $\mu\text{g/L}$ (8.0 %)
23 and 8.2 $\mu\text{g/L}$ (13.8 %). No acute toxicity tests were conducted by the authors. Therefore, an acute
24 chronic ratio could not be derived for anthracene.

3.3.3 Fluoranthene

Fluoranthene has been tested in life-cycle toxicity tests with the freshwater cladoceran, *D. magna* (Spehar et al., 1999) and the saltwater mysid, *A. bahia* (U.S. EPA, 1978, Spehar et al., 1999), and early life-stage tests have been conducted with the fathead minnow (Spehar et al., 1999) (Table 3-1). No effects were observed with *D. magna* at $\leq 17 \mu\text{g/L}$, but growth was reduced 17% at $35 \mu\text{g/L}$ and 25% at $73 \mu\text{g/L}$. There were 37% fewer young per adult at $73 \mu\text{g/L}$ and no daphnids survived at $148 \mu\text{g/L}$. An early life-stage toxicity test conducted with the fathead minnow showed no effects at $\leq 10.4 \mu\text{g/L}$, but reduced survival (67%) and growth (50%) at $21.7 \mu\text{g/L}$.

Saltwater mysids (*A. bahia*) were tested in two life-cycle toxicity tests. In the first test the mysids were exposed to fluoranthene for 28 days (U.S. EPA, 1978). There was no effect on survival or reproduction (growth was not measured) in concentrations ranging from $5\text{--}12 \mu\text{g/L}$. At a fluoranthene concentration of $21 \mu\text{g/L}$, survival was reduced 26.7% and reproduction 91.7%, relative to the controls. At the highest concentration of fluoranthene, $43 \mu\text{g/L}$, all *A. bahia* died. In the second test, *A. bahia* were exposed to fluoranthene for 31 days (Spehar et al., 1999). Effect concentrations were similar to those in the U.S. EPA (1978) test. *A. bahia* were not affected at fluoranthene concentrations from $0.41\text{--}11.1 \mu\text{g/L}$. At the highest concentration tested, $18.8 \mu\text{g/L}$, survival was reduced 23% relative to controls and there was no reproduction. Reproduction was reduced by 77% in $11.1 \mu\text{g/L}$, but this was not significantly different from controls even at $\alpha=0.1$.

The difference between acute and chronic sensitivity to fluoranthene varied minimally between species (Table 3-2). Three species mean ACRs are available for fluoranthene: 4.78 for *D. magna*, 4.60 for *P. promelas*, and 2.33 for *A. bahia*.

3.3.4 Phenanthrene

Phenanthrene has been tested in life-cycle toxicity tests with *D. magna* and *A. bahia* and an early life-stage test has been conducted with rainbow trout (*O. mykiss*) (Table 3-1). There were no effects of phenanthrene on *D. magna* at $\leq 57 \mu\text{g/L}$, but survival was reduced 83% and reproduction 98% at $163 \mu\text{g/L}$ (Call et al., 1986). In a test with *O. mykiss*, no effects were observed at $5 \mu\text{g/L}$. The percentage of abnormal and dead fry at hatch was significantly increased at the highest exposure concentration of $66 \mu\text{g/L}$ and survival of hatched fry was reduced with increase in exposure concentration (Call et al., 1986). Mortality was 41, 48, 52 and 100% at 8, 14, 32, and $66 \mu\text{g/L}$, respectively. Wet weight was reduced 33, 44, and 75% at 8, 14 and $32 \mu\text{g/L}$, respectively.

A life-cycle toxicity test with *A. bahia* exposed to phenanthrene showed that the effect concentrations were similar to those that affected *O. mykiss* (Kuhn and Lussier, 1987)(Table 3-1). Survival, growth and reproduction were not affected at $\leq 5.5 \mu\text{g/L}$. However, at the highest test concentration of phenanthrene ($11.9 \mu\text{g/L}$), all mysids died.

The difference between acute and chronic sensitivity to phenanthrene varied minimally between *D. magna* (PAH-specific ACR= 1.21), *O. mykiss* (ACR=7.90) and *A. bahia* (ACR= 3.33). The ACR for *O. mykiss* (Call et al., 1986) was derived using the EC50 for immobilization ($50 \mu\text{g/L}$) and not the 96-hour LC50 of $375 \mu\text{g/L}$ as was required in Stephan et al. (1985).

3.3.5 Pyrene

A life-cycle toxicity test with *A. bahia* exposed to pyrene was conducted by Champlin and Poucher (1992d). There were no effects at $3.82 \mu\text{g/L}$, but $20.9 \mu\text{g/L}$ reduced survival 37% and no mysids survived at the next higher concentration of $38.2 \mu\text{g/L}$ (Table 3-1). Reproduction was significantly reduced in $\geq 5.37 \mu\text{g/L}$. The ACR for from this test with pyrene is 6.24.

3.3.6 Naphthalene

Fathead minnows were exposed to naphthalene in an early life-stage toxicity test (DeGraeve et al., 1982). Hatching of fry was significantly reduced in 4.38 and 8.51 $\mu\text{g/L}$ and none were alive in these concentrations at the end of the 30-day test. Weight and length of fish surviving the test were significantly reduced in 0.85 and 1.84 $\mu\text{g/L}$. No significant effects were detected in concentrations ≤ 0.45 $\mu\text{g/L}$. Control survival was only 42%, which does not meet requirements according to the American Society of Testing and Materials (ASTM)(1998). Also, the carrier methanol was absent from the control and it was diluted in proportion to the dilution of naphthalene in other treatments. These data are summarized in the text for completeness, but the ACR of 12.7, chronic value of 0.62 $\mu\text{g/L}$, and 96-hour LC50 of 7.9 $\mu\text{g/L}$ for naphthalene are not included in Tables 3-1 and 3-2.

The calanoid copepod (*Eurytemora affinis*) was exposed to 14.21 $\mu\text{g/L}$ naphthalene, 15.03 $\mu\text{g/L}$ 2-methylnaphthalene, 8.16 $\mu\text{g/L}$ 2,6-dimethylnaphthalene and 9.27 $\mu\text{g/L}$ 2,3,5-trimethylnaphthalene in life-cycle toxicity tests (Ott et al., 1978). Survival and reproduction were affected by each of the naphthalenes, but ACRs could not be derived because the duration of the acute test was too short (24 hours) according to guidelines (Stephan et al., 1985), and no other concentrations were tested chronically.

3.3.7 Derivation of the Final Acute Chronic Ratio

The FACR for the six PAHs is 4.16. This FACR is the geometric mean of all species mean ACRs for *Daphnia* (2.41), *Paratanytarsus* (6.68), *Pimephales* (2.61), *Oncorhynchus* (7.90), *Americamysis* (3.59), and *Cyprinodon* (4.37).

3.4 APPLICABILITY OF THE WQC AS THE EFFECTS CONCENTRATION FOR BENTHIC ORGANISMS

The use of the FCV as the effects concentration for calculation of ESGs assumes that benthic (infaunal and epibenthic) species, taken as a group, have sensitivities similar to all aquatic (benthic and water column) species used to derive the WQC FCV. The data supporting the reasonableness of this assumption over all chemicals for which there were published or draft WQC documents were presented in Di Toro et al. (1991), and the "Technical Basis for the Derivation of Equilibrium partitioning Sediment Guidelines (ESGs) for the Protection of Benthic Species: Nonionic Organics" (U.S. EPA, 2000a). The conclusion of similarity of sensitivity was supported by comparisons between (1) acute values for the most sensitive benthic species and acute values for the most sensitive water column species for all chemicals; (2) acute values for all benthic species and acute values for all species in the WQC documents across all chemicals after standardizing the LC50 values; (3) FAVs calculated for benthic species alone and FAVs in the WQC documents; and (4) individual chemical comparisons of benthic species versus all species. The following analysis examines the data on the similarity of sensitivity of benthic and all aquatic species for PAHs.

For PAHs, benthic life-stages were tested for 15 of 20 freshwater genera and 21 out of 29 saltwater genera (Appendix C). An initial test of the difference between the freshwater and saltwater FAVs for all species (water column and benthic) exposed to PAHs was performed using the Approximate Randomization (AR) Method (Noreen, 1989). The AR Method tests the significance level of a test statistic when compared to a distribution of statistics generated from many random subsamples. The test statistic in this case was the difference between the freshwater FAV (computed from the GMAVs at a K_{ow} of 1.0 for combined water column and benthic for freshwater aquatic life) and the saltwater FAV (computed from the GMAVs at a K_{ow} of 1.0 for combined water column and benthic for saltwater aquatic life) (Appendix C). In the AR Method, the freshwater and the saltwater GMAVs

1 at a K_{ow} of 1.0 were combined into one dataset. The dataset was shuffled, then separated back so that
2 randomly generated "freshwater" and "saltwater" FAVs could be computed. The LC50 values were
3 re-separated such that the number of GMAVs at a K_{ow} of 1.0 used to calculate the sample FAVs were
4 the same as the number used to calculate the original FAVs. These two FAVs were subtracted and the
5 difference used as the sample statistic. This was done iteratively so that the sample statistics formed a
6 probability distribution representative of the population of FAV differences (Figure 3-2A). The test
7 statistic was compared to this distribution to determine its level of significance. The null hypothesis
8 was that the GMAVs at a K_{ow} of 1.0 that comprise the freshwater and saltwater data bases were not
9 different. If this was true, the difference between the actual freshwater and saltwater FAVs should be
10 common to the majority of randomly generated FAV differences. For PAHs, the test-statistic occurred
11 at the 93.5 percentile of the generated FAV differences (Table 3-3). This percentile suggests that
12 saltwater genera may be somewhat more sensitive than freshwater genera as illustrated in Figure 3-1
13 and Appendix C. However, since the probability was less than 95% in the AR analysis, the null
14 hypothesis of no significant difference in sensitivity for freshwater and saltwater species was accepted
15 (Table 3-3).

16 Since freshwater and saltwater species showed no significant differences in sensitivity, the AR
17 Method was applied jointly for the analysis of the difference in sensitivity for benthic and all aquatic
18 organisms (benthic and water column species are always combined to derive WQC, therefore, the
19 complete GMAV dataset is hereafter referred to as "WQC"). Using the criteria in U.S. EPA (2000a),
20 each life stage of each test organism, hence each GMAV at a K_{ow} of 1.0, was assigned a habitat
21 (Appendix C). The test statistic in this case was the difference between the WQC FAV, computed
22 from the WQC GMAVs at a K_{ow} of 1.0, and the benthic FAV, computed from the benthic organism
23 GMAVs at a K_{ow} of 1.0. The approach used to conduct this analysis was slightly different than that
24 used in the previous test for freshwater and saltwater GMAVs. The difference was that freshwater and

1 saltwater GMAVs in the first test represented two separate groups. In this test, the GMAVs at a K_{ow} of
2 1.0 for benthic organisms were a subset of the GMAVs at a K_{ow} of 1.0 in the entire WQC dataset. In
3 the AR analysis for this test, the number of data points coinciding with the number of benthic
4 organisms were selected from the WQC dataset to compute each "benthic" FAV. The original WQC
5 FAV and the "benthic" FAV were then used to compute the difference statistic. This was done
6 iteratively and the distribution that results was representative of the population of FAV difference
7 statistics. The test statistic was compared to this distribution to determine its level of significance. The
8 probability distributions of the computed FAV differences are shown in Figure 3-2B. The test statistic
9 for this analysis occurred at the 82.8 percentile and the null hypothesis of no difference in the
10 sensitivities between benthic species and species used to derive the WQC FCV was accepted (Table 3-
11 3). This analysis supports the derivation of the FCV for PAHs based on all GMAVs at a K_{ow} of 1.0.
12

13 3.5 DERIVATION OF FCVs

15 3.5.1 Derivation of the FCV at a K_{ow} of 1.0

17 The FCV is the value that should protect 95% of the tested species. The FCV is the quotient of
18 the FAV and the FACR for the substance. The FAV is an estimate of the acute LC50 or EC50
19 concentration corresponding to a cumulative probability of 0.05 for the genera from eight or more
20 families for which acceptable acute tests have been conducted on the substance. The ACR is the mean
21 ratio of acute to chronic toxicity for three or more species exposed to the substance that meets
22 minimum database requirements. For more information on the calculation of ACRs, FAVs, and FCVs
23 see the U.S. EPA National WQC Guidelines (Stephan et al., 1985).

24 The FCV at a K_{ow} of 1.0 for PAHs is derived using the GMAVs at a K_{ow} of 1.0 from water-

only acute toxicity tests (Appendix C) to calculate the FAV at a K_{ow} of 1.0 which is then divided by the Final ACR.

The FAV at a K_{ow} of 1.0 is calculated using the GMAVs at a K_{ow} of 1.0 of 7.66 $\mu\text{mol/g}$ octanol for *Americamysis*, 8.50 $\mu\text{mol/g}$ octanol for *Grandidierella*, 9.80 $\mu\text{mol/g}$ octanol for *Crangon*, 11.0 $\mu\text{mol/g}$ octanol for *Oncorhynchus*, and the number of genera tested ($N = 49$). The Final Acute Value at a K_{ow} of 1.0 is 9.32 $\mu\text{mol/g}$ octanol. This FAV is greater than the GMAVs of the two most acutely sensitive genera as would be expected given the calculation procedure and the presence of 31 GMAVs.

The FAV at a K_{ow} of 1.0 of 9.32 $\mu\text{mol/g}$ octanol is divided by the Final ACR of 4.16 to obtain a FCV at a K_{ow} of 1.0 of 2.24 $\mu\text{mol/g}$ octanol (Table 3-3). Because nonionic organic chemicals partition similarly into octanol and lipid of organisms, the FCV at a K_{ow} of 1.0 in $\mu\text{mol/g}$ octanol approximately equals tissue-based "acceptable" concentration of about 2.24 $\mu\text{mol/g}$ lipid.

3.5.2 Derivation of the PAH-Specific FCVs

The PAH-specific FCVs ($\mu\text{g/L}$) (Table 3-4) are calculated from the FCV at a K_{ow} of 1.0 ($\mu\text{mol/g}$ octanol), the slope of the K_{ow} - K_{oc} relationship, the universal narcotic slope of the K_{ow} -acute toxicity relationship, and the PAH-specific K_{ow} values (Equation 3-1, 3-2, and 3-3).

$$\log_{10}\text{PAH-specific FCV} = (\text{slope}) * \log_{10}K_{ow} + \log_{10}\text{FCV at a } K_{ow} \text{ of } 1.0 \quad (3-1)$$

$$\log_{10}\text{PAH-specific FCV} = -0.945 \log_{10}K_{ow} + \log_{10}(2.24) \quad (3-2)$$

$$\log_{10}\text{PAH-specific FCV } (\mu\text{mol/L}) = 1000(\text{antilog}(-0.945\log_{10}K_{ow} + 0.3502)) \quad (3-3)$$

SECTION 4

DERIVATION OF ESGs

4.1 DERIVATION OF POTENCIES FOR INDIVIDUAL PAHs IN SEDIMENTS ($C_{OC,PAH,FCV}$)

The critical concentration of a PAH in sediment ($C_{OC,PAH,FCV}$) that is related to the FCV is derived following the EqP method (U.S. EPA, 2000a; Di Toro et al., 1991) because the interstitial water-sediment partitioning of PAHs follows that of other nonionic organic chemicals. Therefore, a sediment effects concentration for any measure of effect can be derived from the product of the water-only effects concentration for that effect and the K_{OC} for that particular PAH. The use of K_{OC} to derive a sediment effects concentration for PAHs is applicable because partitioning for these chemicals is primarily determined by the organic carbon concentration of the sediment.

The partitioning equation between the organic carbon-normalized sediment concentration, C_{OC} ($\mu\text{mol/g}_{OC} = \text{mmol/kg}_{OC}$), and the free interstitial water concentration, C_d (mmol/L), is given by the equation

$$C_{OC} = K_{OC} C_d \quad (4-1)$$

where K_{OC} (L/kg_{OC}), defined above, can be calculated from a K_{OW} obtained from SPARC (Hilal et al., 1994) using the following equation from Di Toro (1985)

$$\log_{10} K_{OC} = 0.00028 + 0.983 \log_{10} K_{OW} \quad (4-2)$$

C_{OC,PAH_i,FCV_i} for individual PAHs are then calculated using Equation 4-1 with the FCV as the water concentration

$$C_{OC,PAH_i,FCV_i} = K_{OC} FCV_i \quad (4-3)$$

Since K_{OC} is presumed to be independent of sediment type for nonionic organic chemicals, so also is C_{OC,PAH_i,FCV_i} .

Table 3-4 contains the C_{OC,PAH_i,FCV_i} ($\mu\text{g/g}_{OC}$) for 74 PAHs found in sediments, including the 34 PAHs (in bold) analyzed by the U.S. EPA in their EMAP program (U.S. EPA, 1996B; 1998).

C_{OC,PAH_i,FCV_i} values for PAHs not in Table 3-4 can be calculated in a similar manner (see Section 6.2 for discussion on the PAHs to which the ESG applies). The range in the C_{OC,PAH_i,FCV_i} values for the 74 PAHs listed in Table 3-4, which were derived using only data for PAHs is from 349 to 1435 $\mu\text{g/g}_{OC}$. In contrast, the range of the same value, termed the $C_{s,OC}$ by Di Toro and McGrath (2000), was about the same (766 to 1887 $\mu\text{g/g}_{OC}$) for the 23 PAHs when derived by using the database for narcotic chemicals with a PAH correction.

4.2 DERIVATION OF THE ESG FOR PAH MIXTURES

The correct derivation of the ESG for a mixture of PAHs is based on the approximate additivity of narcotic chemicals in water and tissue (Di Toro et al., 2000; Section 2.9 of this document) and in sediment (Section 5.2). Because WQC and ESGs are based on FCVs they are not intended to cause toxicity to most species, the term toxic unit could be misleading. Therefore, we refer to the quotient of the concentration of a specific chemical in water and its WQC FCV as water quality criteria toxic units ($WQCTU_{FCV_i}$). Similarly, the quotient of the sediment concentration for a specific PAH (C_{OC,PAH_i}) and

Common Name, Scientific Name	Test Conditions				References
	Test Duration (hr)	Method ^a	Concentration ^b	No. of Data Points ^c	
Sheepshead minnow, <i>Cyprinodon variegatus</i>	96	FT	M	2	Ward et al., 1981; Battelle, 1987
Total Data Points				736 (796)	

^aMethod: S=static, FT=flow-through, R=renewal

^bConcentration: U=unmeasured (nominal), M=chemical measured, I=initial

^cNumber of data points used; ()=number of data before screening for concentration > solubility and outliers.

Common Name, Scientific Name	Test Conditions				References
	Test Duration (hr)	Method ^a	Concentration ^b	No. of Data Points ^c	
Mysid, <i>Americamysis bahia</i>	96	FT	M	8(9)	Battelle, 1987; Champlin and Poucher, 1992a; Horne et al., 1983; EG&G Bionomics, 1978; U.S. EPA, 1978; Kuhn and Lussier, 1987; Thursby, 1991b
Grass shrimp, <i>Palaemonetes pugio</i>	96	R	U	2	Battelle, 1987; Thursby et al., 1989a
Grass shrimp, <i>Palaemonetes pugio</i>	96	S	U	4	Champlin and Poucher, 1992a; Horne et al., 1983; Thursby, 1991b; Tatem et al., 1978
Grass shrimp, <i>Palaemonetes pugio</i>	96	FT	M	1	Battelle, 1987
Grass shrimp, <i>Palaemonetes pugio</i>	96	S	M	1	Tatem, 1977
Crab, <i>Portunus pelagicus</i>	96	S	M	4	Mortimer and Connell, 1994
Inland silverside, <i>Menidia beryllina</i>	96	R	U	1	Thursby et al., 1989a
Inland silverside, <i>Menidia beryllina</i>	96	S	U	7(8)	Champlin and Poucher, 1992a; Dawson et al., 1977; Horne et al., 1983
Sheepshead minnow, <i>Cyprinodon variegatus</i>	24	S	U	7(8)	Heitmuller et al., 1981
Sheepshead minnow, <i>Cyprinodon variegatus</i>	48	S	U	11(12)	Heitmuller et al., 1981
Sheepshead minnow, <i>Cyprinodon variegatus</i>	96	S	U	13(15)	Heitmuller et al., 1981; U.S. EPA, 1978

Common Name, Scientific Name	Test Conditions				References
	Test Duration (hr)	Method ^a	Concentration ^b	No. of Data Points ^c	
Bluegill, <i>Lepomis macrochirus</i>	96	S	U	36(40)	Pickering and Henderson, 1966; U.S. EPA, 1978; LeBlanc, 1980b; ; Buccafusco et al., 1981; Bently et al., 1975; Dawson et al., 1977.
Tadpole, <i>Rana catesbeiana</i>	96	FT	M	5	Thurston et al., 1985
Clawed toad, <i>Xenopus laevis</i>	48	S	U	5	Slooff and Baerselman, 1980
Mexican axolotl, <i>Ambystoma mexicanum</i>	48	S	U	5	Slooff and Baerselman, 1980
<u>Saltwater</u>					
Annelid worm, <i>Neanthes arenaceodentata</i>	96	S	U	4(5)	Horne et al., 1983; Rossi and Neff, 1978
Annelid worm, <i>Neanthes arenaceodentata</i>	96	R	U	(1)	Thursby et al., 1989a
Copepod, <i>Nitocra spinipes</i>	96	S	I	6	Bengtsson et al., 1984
Amphipod, <i>Leptocheirus plumulosus</i>	96	FT	M	4	Swartz, 1991a; Champlin and Poucher, 1992a; Boese et al., 1997
Mysid, <i>Americamysis bahia</i>	96	S	U	20(23)	U.S. EPA, 1978; Champlin and Poucher, 1992a; Zarogian et al., 1985
Mysid, <i>Americamysis bahia</i>	96	S	M	1	EG&G Bionomics, 1982
Mysid, <i>Americamysis bahia</i>	96	R	U	1 8(9)	Thursby et al., 1989b

Common Name, Scientific Name	Test Conditions				References
	Test Duration (hr)	Method ^a	Concentration ^b	No. of Data Points ^c	
Mosquitofish, <i>Gambusia affinis</i>	24	S	U	(3)	Thurston et al., 1985
Mosquitofish, <i>Gambusia affinis</i>	48	S	U	(3)	Thurston et al., 1985
Mosquitofish, <i>Gambusia affinis</i>	96	FT	M	5(6)	Thurston et al., 1985; Wallen et al., 1957
Mosquitofish, <i>Gambusia affinis</i>	96	S	U	3	Wallen et al., 1957
Guppy, <i>Poecilia reticulata</i>	24	S	U	(1)	Pickering and Henderson, 1966
Guppy, <i>Poecilia reticulata</i>	48	S	U	10(11)	Slooff et al., 1983; Pickering and Henderson, 1966
Guppy, <i>Poecilia reticulata</i>	96	S	U	4	Slooff et al., 1983
Bluegill, <i>Lepomis macrochirus</i>	24	S	U	18(19)	Pickering and Henderson, 1966; Buccafusco et al., 1981; Bently et al., 1975
Bluegill, <i>Lepomis macrochirus</i>	24	FT	M	1	Call et al., 1983
Bluegill, <i>Lepomis macrochirus</i>	48	FT	M	1	Call et al., 1983
Bluegill, <i>Lepomis macrochirus</i>	48	S	U	6(7)	Pickering and Henderson, 1966; Bently et al., 1975
Bluegill, <i>Lepomis macrochirus</i>	96	FT	M	8	Thurston et al., 1985; Bently et al., 1975; Call et al., 1983; Holcombe et al., 1987

Common Name, Scientific Name	Test Conditions				References
	Test Duration (hr)	Method ^a	Concentration ^b	No. of Data Points ^c	
Fathead minnow, <i>Pimephales promelas</i>	48	FT	M	8	Ahmad et al., 1984
Fathead minnow, <i>Pimephales promelas</i>	96	FT	M	141(146)	Veith et al., 1983; Thurston et al., 1985; Holcombe et al., 1987; Ahmad et al., 1984; Dill, 1980; DeGraeve et al., 1982; Alexander et al., 1978; Broderius and Kahl, 1985; Cairns and Nebeker, 1982; Hall et al., 1989; Hall et al., 1984; Call et al., 1985; CLSES, 1984; CLSES, 1985; CLSES, 1986; CLSES, 1988; CLSES, 1990; Kimball, 1978
Fathead minnow, <i>Pimephales promelas</i>	96	S	M	3(4)	Bridie et al., 1979; EG&G Bionomics, 1982; Gendussa, 1990; Horne et al., 1983
Fathead minnow, <i>Pimephales promelas</i>	96	R	U	1	Academy Natural Sci., 1981
Fathead minnow, <i>Pimephales promelas</i>	96	S	U	4	Pickering and Henderson, 1966
Channel catfish, <i>Ictalurus punctatus</i>	96	FT,S	M	7	Thurston et al., 1985; Holcombe et al., 1983; Gendussa, 1990
Medaka, <i>Oryzias latipes</i>	48	S	U	4(5)	Slooff et al., 1983
American flagfish, <i>Jordanella floridae</i>	24	FT	M	6	Smith et al., 1991
American flagfish, <i>Jordanella floridae</i>	48	FT	M	6	Smith et al., 1991
American flagfish, <i>Jordanella floridae</i>	96	FT	M	6	Smith et al., 1991

Common Name, Scientific Name	Test Conditions				References
	Test Duration (hr)	Method ^a	Concentration ^b	No. of Data Points ^c	
Bleak, <i>Alburnus alburnus</i>	96	S	I	7	Bengtsson et al., 1984
Goldfish, <i>Carasius auratus</i>	24	S	M	26(28)	Bridie et al., 1979
Goldfish, <i>Carasius auratus</i>	24	S	U	5(6)	Pickering and Henderson, 1966
Goldfish, <i>Carasius auratus</i>	24	FT	M	1(2)	Brenniman et al., 1976
Goldfish, <i>Carasius auratus</i>	96	S	U	4	Pickering and Henderson, 1966
Goldfish, <i>Carasius auratus</i>	96	FT	M	1(2)	Brenniman et al., 1976
Goldfish, <i>Carasius auratus</i>	48	S	U	5(6)	Pickering and Henderson, 1966
Goldfish, <i>Carasius auratus</i>	48	FT	M	1(2)	Brenniman et al., 1976
Golden orfe, <i>Leuciscus idus melanotus</i>	24	S	i(ns)	26	Juhnke and Ludemann, 1978
Fathead minnow, <i>Pimephales promelas</i>	24	S	U	6	Pickering and Henderson, 1966
Fathead minnow, <i>Pimephales promelas</i>	24	FT	M	8	Ahmad et al., 1984
Fathead minnow, <i>Pimephales promelas</i>	48	S	U	11	Pickering and Henderson, 1966

Common Name, Scientific Name	Test Conditions				References
	Test Duration (hr)	Method ^a	Concentration ^b	No. of Data Points ^c	
Brine shrimp, <i>Artemia salina</i>	24	S	N	32(34)	Abernethy et al., 1988; Abernethy et al., 1986
Crayfish, <i>Orconectes immunis</i>	96	FT	M	6	Thurston et al., 1985; Holcombe et al., 1987
Mosquito, <i>Aedes aegypti</i>	48	S	U	5	Slooff et al., 1983
Mosquito, <i>Culex pipiens</i>	48	S	U	5	Slooff et al., 1983
Midge, <i>Tanytarsus dissimilis</i>	48	S	M	9	Thurston et al., 1985; Call et al., 1983
Rainbow trout, <i>Oncorhynchus mykiss</i>	48	FT	M	7	Holcombe et al., 1987; Call et al., 1983
Rainbow trout, <i>Oncorhynchus mykiss</i>	24	FT	M	6	Call et al., 1983
Rainbow trout, <i>Oncorhynchus mykiss</i>	24	S	U	1(2)	Bently et al., 1975
Rainbow trout, <i>Oncorhynchus mykiss</i>	48	S	U	6	Slooff et al., 1983; Bently et al., 1975
Rainbow trout, <i>Oncorhynchus mykiss</i>	96	FT	M	22	Thurston et al., 1985; Call et al., 1983; Holcombe et al., 1987; Call et al., 1986; DeGraeve et al., 1982; Hodson et al., 1988
Rainbow trout, <i>Oncorhynchus mykiss</i>	96	S	M	1	Horne et al., 1983
Rainbow trout, <i>Oncorhynchus mykiss</i>	96	S	U	1	Bently et al., 1975

Appendix A. Individual datasets which comprise the acute lethality data base. Table from Di Toro et al. (2000).

Common Name, Scientific Name	Test Conditions			No. of Data Points ^c	References
	Test Duration (hr)	Method ^a	Concentration ^b		
<u>Freshwater</u>					
Paramecium, <i>Tetrahymena ellioti</i>	24	S	U	10(12)	Rogerson et al., 1983
Hydra, <i>Hydra oligactis</i>	48	S	U	5	Slooff et al., 1983
Snail, <i>Lymnae stagnalis</i>	48	S	U	5	Slooff et al., 1983
Cladoceran, <i>Daphnia cucullata</i>	48	S	U	5	Canton and Adema, 1978
Cladoceran, <i>Daphnia magna</i>	24	S	U	21(28)	LeBlanc, 1980a
Cladoceran, <i>Daphnia magna</i>	48	S	U	72(78)	Abernethy et al., 1988; U.S. EPA, 1978; Canton and Adema, 1978 Rogerson et al., 1983; Bringman and Kuhn, 1959; Eastman et al., 1984; Dill, 1980
Cladoceran, <i>Daphnia magna</i>	48	S	U	19	EG&G Bionomics, 1982; Thurston et al., 1985; Adema, 1978; Oris et al., 1991; Brooke, 1991; Millemann et al., 1984; Munkrittrick et al., 1991
Cladoceran, <i>Daphnia magna</i>	48	FT,R	M	1(2)	EG&G Bionomics, 1982; Brooke, 1994
Cladoceran, <i>Daphnia pulex</i>	48	S	M	(1)	Trucco et al., 1983
Cladoceran, <i>Daphnia pulex</i>	48	S	U	6	Canton and Adema, 1978; Passino and Smith, 1987

Table 6-3. Teratogenic and carcinogenic effects of benzo(a)pyrene (BaP) and anthracene on freshwater and saltwater fishes. Measured concentrations of exposure are converted to sediment concentrations (C_{OC}) likely to result in the equivalent effect using EqP and SAR methodology.

Organism	Chemical	$\log_{10} K_{OW}$	$\log K_{OC}$	Measured C_d^a ($\mu\text{g/L}$)	C_d -derived C_{OC} ($\mu\text{g/g}_{OC}$)	Measured C_{ORG}^b ($\mu\text{g/g}$)	f_{Lipid}	C_L^b ($\mu\text{g/g Lipid}$)	C_L -derived C_{OC} ($\mu\text{g/g}_{OC}$)	References
TERATOGENIC EFFECTS										
<u>FRESHWATER</u>										
Fathead minnow eggs	Anthracene	4.53	4.46	-	-	8.8	0.06	147	219	Hall and Oris, 1991
Topminnows	BaP	6.11	6.00	>3.81 ^c (1,000)	>3810	9	0.06	150	256	Goddard et al., 1987
Rainbow trout eggs	BaP	6.11	6.00	0.21	210	1.9	0.05	38.6	66	Hannah et al., 1982 Hose et al., 1984
<u>SALTWATER</u>										
English sole eggs	BaP	6.11	6.00	-	-	157	0.03	5233 ^d	8,937 ^d	Hose et al., 1981
Sand sole eggs	BaP	6.11	6.00	0.10	100	2.1	0.03	70	120	Hose et al., 1982
Calif. grunion eggs	BaP	6.11	6.00	>3.81 (5)	>3810	1	0.03	33.3	57	Winkler et al., 1983
Calif. grunion eggs	BaP	6.11	6.00	>3.81 (24)	>3810	10.5	0.03	350	598	Winkler et al., 1983
Calif. grunion eggs	BaP	6.11	6.00	>3.81 ^c (869)	>3810	20.0	0.03	666	1,137	Winkler et al., 1983
CARCINOGENIC EFFECTS										
<u>FRESHWATER</u>										
Japanese medaka	BaP	6.11	6.00	>3.81 ^c (261)	>3840	-	-	-	-	Hawkins et al., 1988, 1990
guppy	BaP	6.11	6.00	>3.81 ^c (209)	>3840	-	-	-	-	Hawkins et al., 1988, 1990

^a If the concentration of BaP exceeded its solubility of 3.81 $\mu\text{g/L}$, the published concentration in water is listed in parenthesis with the solubility of 3.81 $\mu\text{g/L}$ listed above as the concentration of exposure. Therefore the maximum C_{OC} value for these exposures is 3840 $\mu\text{g BaP/g}_{OC}$.

^b Concentrations in eggs on a wet weight basis are converted to concentrations on a lipid basis using lipid concentrations (f_{Lipid}) from Table 1 in Kamler (1992).

^c Water concentrations of BaP were not stable throughout the duration of the experiment.

^d The solubility of BaP in water theoretically limits the maximum concentration in eggs to ~3,840 $\mu\text{g/g lipid}$ and in sediments to ~3,840 $\mu\text{g/g}_{OC}$, but metabolites of BaP will likely be included in radio-labeled quantification of total BaP equivalents.

Table 6-2. PAH measured in various sediment monitoring programs. See Di Toro and McGrath (2000) for data sources.

Parameter	NOAA	SFEI	San Diego	Southern California	NY/NJ REMAP ^A	Virginian EMAP ^B	Elliott Bay	Carolinian EMAP	Louisian EMAP
Acenaphthene	x	x	x	x	x	x	x	x	x
Acenaphthylene	x	x	x	x	x	x	x	x	x
Anthracene	x	x	x	x	x	x	x	x	x
Chrysene	x	x	x	x	x	x	x	x	x
Fluoranthene	x	x	x	x	x	x	x	x	x
Fluorene	x	x	x	x	x	x	x	x	x
naphthalene	x	x	x	x	x	x	x	x	x
phenanthrene	x	x	x	x	x	x	x	x	x
pyrene	x	x	x	x	x	x	x	x	x
Benzo(k)fluoranthene	x	x	x	x	x	x	x	x	x
Benzo(b)fluoranthene	x	x	x	x	x	x	x	x	x
Benzo(a)pyrene	x	x	x	x	x	x	x	x	x
Benzo(a)anthracene	x	x	x	x	x	x	x	x	x
Benzo(e)pyrene	x	x	x	x	x	x	x	x	x
Benzo(g,h,i)perylene	x	x	x	x	x	x	x	x	x
Dibenz(a,h)anthracene	x	x	x	x	x	x	x	x	x
2,6-dimethylnaphthalene	x	x	x	x	x	x	x	x	x
Indeno(1,2,3-cd)pyrene	x	x	x	x	x	x	x	x	x
1-methylnaphthalene	x	x	x	x	x	x	x	x	x
2-methylnaphthalene	x	x	x	x	x	x	x	x	x
perylene	x	x	x	x	x	x	x	x	x
1-methylphenanthrene	x	x	x	x	x	x	x	x	x
2,3,5-trimethylnaphthalene	x	x	x	x	x	x	x	x	x
2-methylanthracene							x		
2-methylphenanthrene		x					x		
3,6-dimethylphenanthrene							x		
9-methylanthracene		x					x		
9,10-dimethylanthracene							x		
C1-benzo(a)anthracenes /chrysenes							x	x	x
C2-benzo(a)anthracenes /chrysenes							x	x	x
C3-benzo(a)anthracenes /chrysenes								x	x
C4-benzo(a)anthracenes /chrysenes								x	x
C1-fluoranthenes/pyrenes							x	x	x
C2-fluoranthenes/pyrenes							x		
C1-fluorenes							x	x	x
C2-fluorenes							x	x	x
C3-fluorenes							x	x	x
C1-naphthalenes								x	x
C2-naphthalenes							x	x	x
C3-naphthalenes							x	x	x
C4-naphthalenes							x	x	x
C1-phenanthrenes/anthracenes							x	x	x
C2-phenanthrenes/anthracenes							x	x	x
C3-phenanthrenes/anthracenes							x	x	x
C4-phenanthrenes/anthracenes								x	x
Total Number of PAHs ^B	23	25	23	23	23	23	33 ^C	34	34
Number of data points	640	137	182	40	153	318	30	280	229

^A Benzo(b)fluoranthene and benzo(k)fluoranthene were measured together.

^B A specific C1-PAH was not included in the total if the C1 alkylated PAH series was measured.

For example, 1-methylnaphthalene was not included in the total if the C1-naphthalenes were measured.

^C For this dataset, the C1-Naphthalenes were not measured. As a result, the 1-methylnaphthalene and 2-methylnaphthalene were considered when determining the total number of PAHs.

Table 6-1. Relative Distribution of $\Sigma\text{ESGTU}_{\text{FCV,TOT}}$ to $\Sigma\text{ESGTU}_{\text{FCV,13}}$ and $\Sigma\text{ESGTU}_{\text{FCV,23}}$ for the Combined EMAP Dataset (N=488).

Percentile	$\Sigma\text{ESGTU}_{\text{FCV,TOT}} / \Sigma\text{ESGTU}_{\text{FCV,13}}$	$\Sigma\text{ESGTU}_{\text{FCV,TOT}} / \Sigma\text{ESGTU}_{\text{FCV,23}}$
50	2.75	1.64
80	6.78	2.80
90	8.45	3.37
95	11.5	4.14
99	16.9	6.57

Table 5-3. Chemicals included in the high K_{ow} PAH mixture experiment (Spehar et al., 2000).

Chemical Name	Molecular Weight (g/mol)	$\log_{10} K_{ow}^a$	$\log_{10} K_{oc}^b$	Estimated Solubility ^c ($\mu\text{g/L}$)	Target Sediment Concentration ($\mu\text{mol/g}_{oc}$)	Nominal Water Concentration ^d ($\mu\text{g/L}$)	Solubility Limited Nominal Water Concentration ($\mu\text{g/L}$)
3,6-Dimethylphenanthrene	206.29	5.52	5.42	77.98	42.38	33.12	33.12
2-Ethylanthracene	206.29	5.36	5.27	59.62	39.32	43.94	43.94
2-(tert-butyl)anthracene	234.34	5.88	5.78	33.04	50.91	19.78	19.78
2,3 Benzofluorene	216.28	5.54	5.44	25.30	42.88	33.27	25.30
Benzo(a)anthracene	228.29	5.67	5.58	12.28	45.80	27.70	12.28
Triphenylene	228.30	5.75	5.65	5.110	47.66	24.11	5.110
9-Phenylanthracene	254.33	6.31	6.20	3.640	64.22	10.30	3.640
Benzo(b)fluoranthene	252.32	6.27	6.16	8.280	62.75	10.96	8.280
Benzo(k)fluoranthene	252.32	6.29	6.18	8.350	63.64	10.50	8.350
7,12-Dimethylbenz(a)anthracene	256.35	6.58	6.46	13.41	75.04	6.620	6.620
Benzo(a)pyrene	252.31	6.11	6.00	2.880	57.46	14.38	2.880
3-Methylcholanthrene	268.38	6.76	6.64	3.110	83.92	5.100	3.110
7-Methylbenzo(a)pyrene	266.35	6.54	6.43	1.460	73.37	7.320	1.460
TOTAL PAH- WATER CONCENTRATION					749.4	247.1	173.9

^aPredicted by SPARC in distilled water at 25°C.

^bPredicted from Di Toro et al. (1991).

^cNominal concentration predicted by K_{oc} , regardless of solubility limits; highest concentration only.

^dTarget sediment concentration/ K_{oc} .

Table 5-2. Percent mortality of benthic invertebrates in relation to the Σ ESGTU_{FCV} values of mixtures of polycyclic aromatic hydrocarbons spiked into sediment.

Species ^a	Σ ESGTU _{FCV} PAH Kow <5.5	Σ ESGTU _{FCV} PAH Kow >5.5	Σ ESGTU _{FCV} All PAHs	Percent Mortality	PAH Mixture ^b	Reference
<i>Diporeia</i> sp.	0.01	0.02	0.03	3	fluor, phen, anthr, flu, pyr, chry, b(b)flu, b(e)pyr, b(a)pyr, pery, b(ghi)pery	Landrum et al., 1991
<i>Diporeia</i> sp.	0.21	0.36	0.57	10	fluor, phen, anthr, flu, pyr, chry, b(b)flu, b(e)pyr, b(a)pyr, pery, b(ghi)pery	Landrum et al., 1991
<i>Diporeia</i> sp.	0.49	0.60	1.10	0	fluor, phen, anthr, flu, pyr, chry, b(b)flu, b(e)pyr, b(a)pyr, pery, b(ghi)pery	Landrum et al., 1991
<i>Diporeia</i> sp.	1.37	1.71	3.08	12	fluor, phen, anthr, flu, pyr, chry, b(b)flu, b(e)pyr, b(a)pyr, pery, b(ghi)pery	Landrum et al., 1991
<i>R. abronius</i>	10.32	0	10.3	100	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	5.80	0	5.80	38	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	5.12	0	5.12	8	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	3.25	0	3.25	11	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	2.50	0	2.50	4	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	1.80	0	1.80	2	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	1.42	0	1.42	3	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	2.77	0	2.77	5	anthr; flu	Boese et al., 1999
<i>R. abronius</i>	4.91	5.02	9.93	3	b(a)anthr; flu	Boese et al., 1999
<i>R. abronius</i>	5.88	0	5.88	5	2-methylanthr; flu	Boese et al., 1999
<i>R. abronius</i>	5.71	0	5.71	2	9,10-dimethylanthr; flu	Boese et al., 1999
<i>R. abronius</i>	2.71	2.23	4.94	3	b(b)flu; flu	Boese et al., 1999
<i>R. abronius</i>	2.06	0.79	2.84	2	chr; flu	Boese et al., 1999
<i>R. abronius</i>	0.63	1.57	2.20	1	3,6-dimethylphen; flu	Boese et al., 1999
<i>R. abronius</i>	1.91	25.89	27.8	4	anthr; b(a)anthr; 2-methylanthr; b(b)flu; chr; 3,6-dimethylphen	Boese et al., 1999
<i>R. abronius</i>	0.58	8.03	8.61	5	anthr; b(a)anthr; 2-methylanthr; b(b)flu; chr; 3,6-dimethylphen	Boese et al., 1999
<i>R. abronius</i>	1.55	8.03	9.58	9	anthr; b(a)anthr; 2-methylanthr; b(b)flu; chry; 3,6-dimethylphen; flu	Boese et al., 1999
<i>R. abronius</i>	0.90	3.40	4.30	0	anthr; b(a)anthr; 2-methylanthr; b(b)flu; chry; 3,6-dimethylphen; flu	Boese et al., 1999
<i>A. abdita</i>	5.41	0.64	6.05	7	9,10-dimethylanthr; chry	Burgess et al., 2000
<i>A. abdita</i>	0	2.58	2.58	7	b(a)pyr; cor	Burgess et al., 2000
<i>A. abdita</i>	5.41	3.22	8.63	10	9,10-dimethylanthr; chry; b(a)pyr; cor	Burgess et al., 2000
<i>A. bahia</i>	5.41	0.64	6.05	3	9,10-dimethylanthr; chry	Burgess et al., 2000
<i>A. bahia</i>	0	2.58	2.58	7	b(a)pyr; cor	Burgess et al., 2000
<i>A. bahia</i>	5.41	3.22	8.63	7	9,10-dimethylanthr; chry; b(a)pyr; cor	Burgess et al., 2000

^aTest Species: amphipods: *Diporeia* sp., *Rhepoxynius abronius*, *Ampelisca abdita*; mysids: *Americamysis bahia*

^bPAH Code: ace - acenaphthene; anthr - anthracene; b(a)anthr - benz(a)anthracene; b(a)pyr - benzo(a)pyrene; b(ghi)pery - benzo(ghi)perylene; b(b)flu - benzo(b)fluoranthene; chry - chrysene; cor - coronene; 9,10-dimethylanthr - 9,10-dimethylanthrane; 3,6-dimethylphen - 3,6dimethylphenanthrene; flu - fluoranthene; fluor - fluorene; 2-methylanthr - 2-methylanthrane; pery - perylene; phen - phenanthrene; pyr - pyrene.

<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	22.7	1.63	1890	1390	1.36	Swartz et al., 1990
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	29.4	2.12	2100	1390	1.51	Swartz et al., 1990
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	24.2	1.74	2230	1390	1.60	Swartz et al., 1990
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	> 315	> 22.66 ^D	> 4360	1390	4.04 ^D	DeWitt et al., 1992
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	14.1	1.01	4410	1390	3.17	DeWitt et al., 1992
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	26.6	1.91	3080	1390	2.22	DeWitt et al., 1992
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	19.2	1.38	3150	1390	2.26	DeWitt et al., 1992
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	9.38	0.67	2790	1390	2.01	DeWitt et al., 1992
Mean LC50 ratio =					1.60	Mean LC50 ratio =			1.91

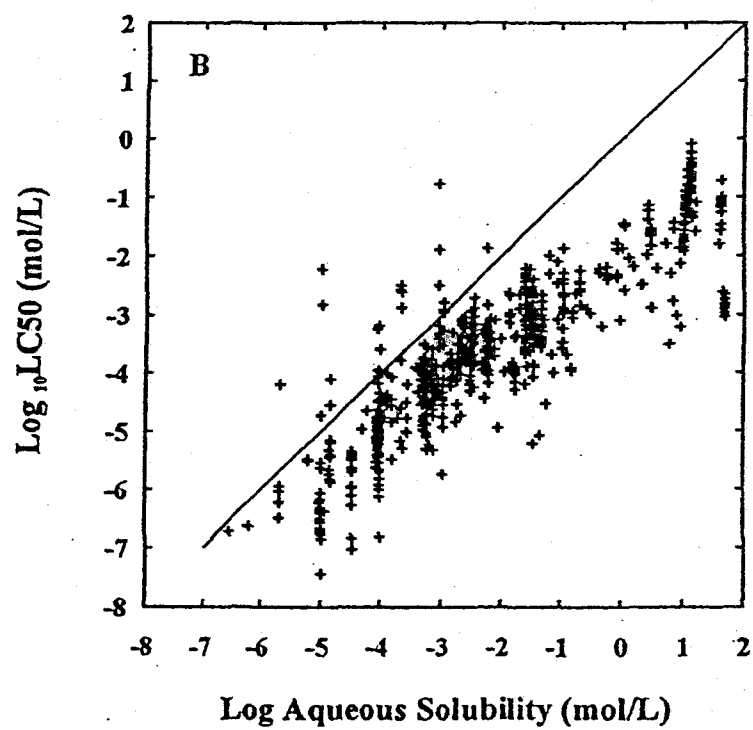
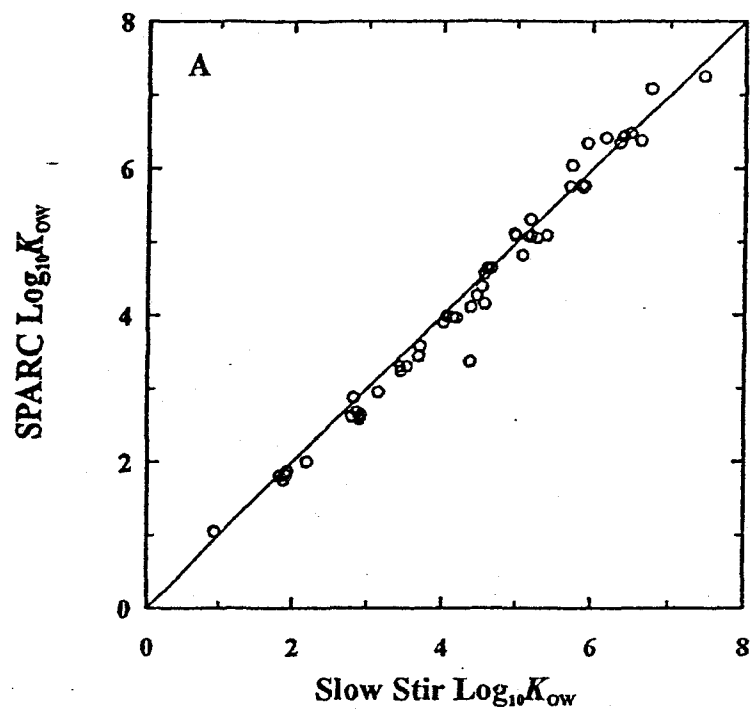
^aTest conditions for water-only toxicity tests: S = static, FT = flow-through, M = measured, 10 = 10-d duration.

^bPredicted LC50 ($\mu\text{g/g}_{\text{oc}}$) = water-only LC50 ($\mu\text{g/L}$) $\times K_{\text{oc}}$ (L/kg_{oc}) $\times 1 \text{ kg}_{\text{oc}}/1000\text{g}_{\text{oc}}$.

^cSediments spiked with fluoranthene by Suedel et al. (1993) were not at equilibrium, therefore, are not included in the mean.

^dSource of organic carbon was fresh plant material, not naturally aged organic matter, therefore, value was not included in the mean.

^e10-day LC50 value from Swartz (2000).



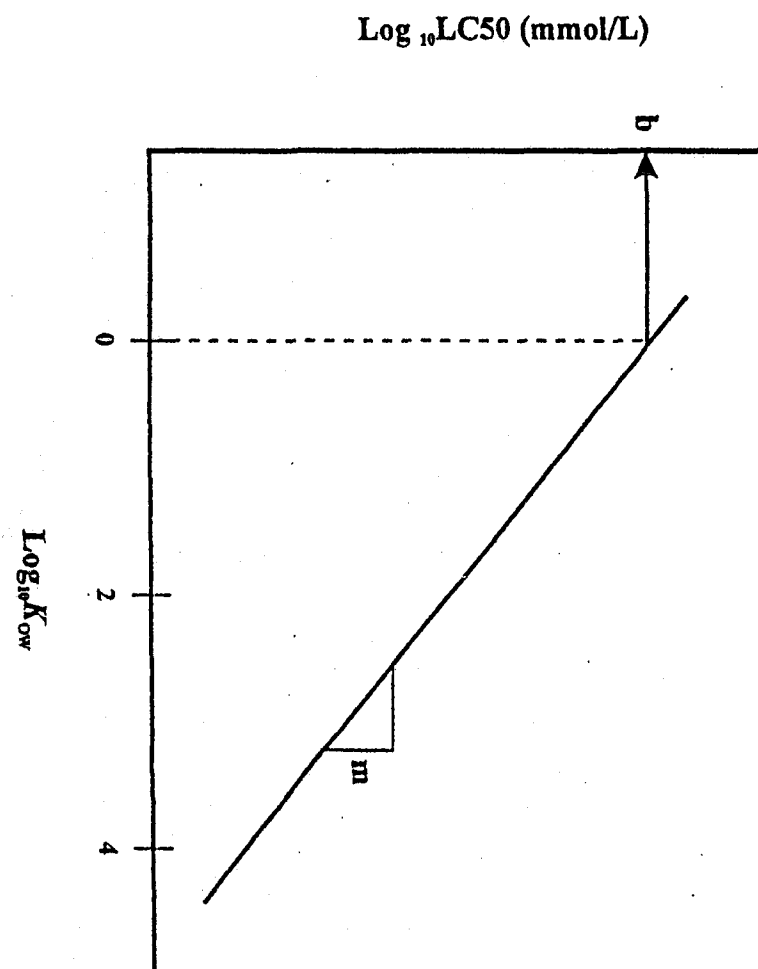


Figure 6-5. Computed solubilities of nine PAHs relative to their 25°C solubilities as a function of temperature. The solid line is the least-squares regression line (Equation 6-10).

are treatments with effects significantly different from controls.

Figure 5-11. Amphipod (*Ampelisca abdita*) abundance versus $\Sigma\text{ESGTU}_{\text{FCV}}$. Vertical line is the ESG of 1.0 $\Sigma\text{ESGTU}_{\text{FCV}}$. Data are from the Virginian and Louisianian province EMAP (U.S. EPA, 1996a,b) and the New York/New Jersey Harbor REMAP (Adams et al., 1996).

Figure 6-1. Comparison of observed $\Sigma\text{ESGTU}_{\text{FCV,TOT}}$ to observed $\Sigma\text{ESGTU}_{\text{FCV,13}}$ from 13 PAHs (A) and $\Sigma\text{ESGTU}_{\text{FCV,23}}$ from 23 PAHs (B) for the combined dataset including U.S. EPA EMAP Louisian and Carolinian Provinces (N=490). The line shows the resulting log-log linear regression equation.

Figure 6-2. Probability distribution of the (A) $\Sigma\text{ESGTU}_{\text{FCV,13}}$ and (B) $\Sigma\text{ESGTU}_{\text{FCV,23}}$ values for each sediment from the entire database. Symbols are as described in text.

Figure 6-3. BaP concentration of 539 sediment samples from the EMAP and Elliot Bay datasets versus the ΣESGU s of 34 PAHs (A) and a probability plot of these BaP concentrations at an $\Sigma\text{ESGU} = 1$ (B). The solid line in both plots is the BaP critical sediment concentration for teratogenic and carcinogenic effects ($57 \mu\text{g/g}_{\text{OC}}$).

Figure 6-4. Anthracene concentration of 539 sediment samples from the EMAP and Elliot Bay datasets versus the ΣESGU s of 34 PAHs (A) and a probability plot of these Anthracene concentrations at an $\Sigma\text{ESGU} = 1$ (B). The solid line in both plots is the Anthracene critical sediment concentration for teratogenic effects ($219 \mu\text{g/g}_{\text{OC}}$).

spiked with a mixture of high K_{ow} PAH. Acute TUs were calculated based on measured sediment PAH concentrations and the GMAV from Appendix C. Asterisks indicate significant reduction compared to the control ($\alpha=0.05$).

Figure 5-7. Response of *H. azteca* exposed for 28 days under flow-through conditions to sediment spiked with a mixture of high K_{ow} PAH. Acute TUs were calculated based on measured sediment PAH concentrations and the GMAV from Appendix C. Asterisks indicate significant reduction compared to the control ($\alpha=0.05$).

Figure 5-8. Survival (after 28 days) and growth (after 10 days) of *H. azteca* expressed on the basis of measured PAH concentrations in tissues (lipid normalized). Effect concentrations were calculated from acute water-only effect data for fluoranthene, methanol, ethanol, and 2-propanone using the narcosis model. Acute TUs were calculated by dividing the lipid-normalized concentration of PAH in tissue by the GMAV, assuming lipid = octanol. The chronic threshold is represented by the GMAV divided by the ACR. Data are from Di Toro et al. (1999).

Figure 5-9. Response of *H. azteca* exposed for 10 days (3 renewals) to sediment spiked with a mixture of high K_{ow} PAH. Acute TUs were calculated based on measured sediment PAH concentrations and the GMAV from Appendix C. Asterisks indicate significant reduction compared to the control ($\alpha=0.05$).

Figure 5-10. Response of *L. plumulosus* exposed for 10 days under static conditions to sediment spiked with a mixture of high K_{ow} PAH. Acute TUs were calculated based on measured sediment PAH concentrations and the GMAV from Appendix C. Asterisks

three sediments per chemical. Sediment types are indicated by open symbols (lowest organic carbon content), doubled symbols (intermediate organic carbon content) and filled symbols (highest organic carbon content). Uncertainty error bars are represented by solid vertical lines (see U.S. EPA, 1999a for source of K_{oc} values).

Figure 5-3. Percent mortality of *Rhepoxynius abronius* in sediments spiked with acenaphthene, phenanthrene, fluoranthene, or pyrene (see Appendix D for data).

Figure 5-4. Percentage rank, based on $ESGTU_{FCVI}$, of the sensitivities of genera of benthic organisms from spiked sediment toxicity tests with individual PAHs.

Figure 5-5. Mortality of the amphipod, *Rhepoxynius abronius*, from tests 10-day sediment toxicity tests with four parent PAHs separately (triangles) and in combination (circles) from (Swartz et al., 1997) versus predicted sediment toxic units (PSTUs). PSTUs are the sediment concentrations in each treatment divided by the predicted PAH-specific sediment LC50 values. The predicted PAH-specific sediment LC50 values are derived from the interstitial water 10-day LC50 values from spiked sediment toxicity tests and the universal narcosis slope to derive the PAH-specific critical tissue concentrations. The geometric mean of the critical tissue concentrations, the universal narcosis slope and the PAH-specific K_{ow} and K_{oc} were used to derive PAH-specific sediment LC50 values. For the mixture experiment the toxic units are the sum of the sediment concentrations for each of the four PAHs divided by their respective PAH-specific sediment LC50 values.

Figure 5-6. Response of *H. azteca* exposed for 10 days under flow-through conditions to sediment

the tested mixtures are as indicated (adopted from Hermens et al., 1984).

Figure 3-1. GMAVs at a $\log_{10}K_{OW}$ of 1.0 from water-only acute toxicity tests using freshwater and saltwater genera versus percentage rank of their sensitivity. Freshwater genera are indicated by open symbols and saltwater genera are indicated by closed symbols.

Figure 3-2. Probability distributions of FAV difference statistics to compare water-only toxicity data from (A) freshwater versus saltwater genera and (B) benthic versus WQC.

Figure 4-1. Probability distribution of the $\Sigma ESGTU_{FCV}$ for PAH mixtures in sediments from coastal and estuarine locations in the United States (NOAA, 1991; Adams et al., 1996; Anderson et al., 1996; Fairey et al., 1996; U.S. EPA, 1996a, b, 1998; Hunt et al., 1998). Horizontal line indicates a toxic unit of 1.0.

Figure 4-2. Probability distribution of the $\Sigma ESGTU_{FCV}$ for PAH mixtures in sediments from all the coastal and estuarine locations in the United States from Figure 4-1 (NOAA, 1991; Adams et al., 1996; Anderson et al., 1996; Fairey et al., 1996; U.S. EPA, 1996a, b, 1998; Hunt et al., 1998). Horizontal line indicates a toxic unit of 1.0.

Figure 5-1. Percent mortality versus predicted interstitial water toxic units for six chemicals and three sediments per chemical. Sediment types are indicated by open symbols (lowest organic carbon content), doubled symbols (intermediate organic carbon content) and filled symbols (highest organic carbon content).

Figure 5-2. Percent mortality versus predicted interstitial water toxic units for seven chemicals and

FIGURES

- Figure 2-1. Schematic diagram of the $\log_{10}\text{LC50}$ versus $\log_{10}K_{\text{OW}}$ relationship. At $\log_{10}K_{\text{OW}} = 0$, $K_{\text{OW}} = 1$, the concentration in water equals the concentration in octanol.
- Figure 2-2. Comparisons of (A) $\log_{10}K_{\text{OW}}$ predicted by SPARC versus measured $\log_{10}K_{\text{OW}}$ using slow stir method and (B) reported $\log_{10}\text{LC50}$ values versus the aqueous solubility estimated by SPARC. The diagonal line represents equality.
- Figure 2-3. Ratios of (A) 48- to 96-hour LC50 values and (B) 24- to 96-hour LC50 values versus $\log_{10}K_{\text{OW}}$. The line in (B) is the regression used to correct the 24-hour LC50 to 96-hour LC50.
- Figure 2-4. $\log_{10}\text{LC50}$ versus $\log_{10}K_{\text{OW}}$ for the indicated species. The line has a constant slope of -0.945 . The y-intercepts vary for each species. Outliers are denoted by a plus symbol (+).
- Figure 2-5. Statistical comparison of slopes fitted to individual species to the universal slope of -0.945 showing (A) the probability that the difference occurred by chance (filled bars) and number of data points in the comparison (hatched bars) for each species in the database, and (B) the deviations of the individual estimates from the universal slope. Abbreviations are based on the first letter of the genus and either the first or second letters of the species names given in Appendix A (e.g., *Aae* = *Aedes aegypti* and *Am* = *Ambystoma mexicanum*).

Figure 2-6. Chemical class comparisons. (A) Residuals from the regression grouped by class with mean \pm 2 standard errors. (B) Residuals grouped by class with chemical class corrections included in the regression.

Figure 2-7. The coefficient of variation of the estimated species-specific body burdens versus the number of data points for that species (A), the log probability plot of the residuals (B), and the residuals versus $\log_{10}K_{ow}$ (C).

Figure 2-8. $\log_{10}LC50$ versus $\log_{10}K_{ow}$ for (A) *L. macrochirus*, (B) *D. pulex*, and (C) *G. affinis*. The line connects the individual estimates of the LC50 values, including the chemical class correction.

Figure 2-9. Comparison of target lipid model, line-of-fit and observed LC50 data for individual PAHs, by species. The PAHs included are: naphthalene (3.36), 1-methylnaphthalene (3.84), 2-methylnaphthalene (3.86), 2-chloronaphthalene (3.88), 1-chloronaphthalene (3.88), acenaphthene (4.01), phenanthrene (4.57), pyrene (4.92), 9-methylanthracene (5.01), fluoranthene (5.08). Number in parentheses = $\log_{10}K_{ow}$. Solid line and filled symbols are for non-halogenated PAHs. Dotted lines and unfilled symbols are for the halogenated (i.e., chlorinated) PAHs. Plus symbols (+) denote outliers. Data are from Di Toro et al. (2000) and were used for toxicity test screening criteria.

Figure 2-10. Predicted and observed body burdens for five species.

Figure 2-11. Additivity of type I narcosis toxicity. Comparison of the observed TU concentrations calculated from four studies to the predicted TU of 1.0. The number of chemicals in

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
<i>Poeciliopsis lucida</i> and <i>Poeciliopsis monacha</i> (1-7 months old)	water; acetone carrier	Lab: (multiple exposures) 3 to 4 exposure periods of 5-20 hours each week	7,12-dimethylbenz(a)-anthracene	5 ppm (per exposure)	7 - 8 months (from initial exposure)	incidence of hepatic tumors = 48%	-	only survivors examined = (55% mortality in 5 ppm treatment) (13% mortality in control)	Schultz and Schultz 1982
<i>Poeciliopsis lucida</i> and <i>Poeciliopsis monacha</i> (1-6 weeks old)	water; acetone carrier	Lab: (multiple exposures) 5 exposures periods of 6 hours each week	7,12-dimethylbenz(a)-anthracene	5 ppm (per exposure)	6 - 7 months	Incidence of hepatic tumors = 41.8%	-	22% mortality in treatment 16% mortality in control Tumor-bearing livers enlarged, yellow-white to greenish and granular.	Schultz and Schultz 1982
Bullheads	Direct skin (river sediment extract)	Lab	Field Mixture ^A	5% RSE painted once per week	18 months	23% of survivors hyperplastic 9% with multiple papillomas	-	Survival of control and experimental fish was 31%.	Black, 1983
Japanese Medaka, <i>Poecilia reticulata</i> (6-10 d old)	Water via Sediment extract re-dissolved in acetone	Lab	Field Mixture ^B	182 ppb TPAH Black River, OH extract; 254 ppb TPAH Fox River, WI extract	24 h	hepatocellular carcinoma - Black River Ex. (2/15 fish); Pancreatic-duct cell adenoma - Fox River Ex. (1/15 fish)	-	No incidence of carcinomas in controls up to 270 days post-exposure; one incidence of lymphoma after 360 days of exposure.	Fabacher et al., 1991
Rainbow trout embryos), <i>Oncorhynchus mykiss</i>	injection of sediment extract into yolk sac	Lab	Field Mixture ^C	Doses ^D : (Exp I) 0.006 g (Exp II) 0.012 g 0.006 g 0.003 g	1 year	Hepatic carcinomas (I) 8.9% (11/123) (II) 8.1% (12/148) 4.0% (5/148) 3.1% (2/65)	-	Note; PCBs also present sediment from Hamilton Harbour	Metcalf et al 1988

Buffalo River, NY; total no. PAHs measured = 13, total no. of carcinogenic PAHs = 6.

Black River, OH. And Fox River, WI; full compliment of measured PAHs.

Hamilton Harbor, ON, Canada; total no. PAHs measured = 13, total no. of carcinogenic PAHs = 6.

Doses are calculated as gram equivalent wet weight of sediment represented by the volume of extract micro-injected into each trout sac-fry.

Appendix F. Carcinogenic effects from laboratory and field exposure to PAHs and PAH mixtures.

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
Japanese Medaka, <i>Oryzias latipes</i> (6-10 d old)	Water; dimethyl-formamide carrier.	Lab; static	BaP	261 µg/L	2 x 6h, 1 week apart	Neoplastic lesions in livers and other tissues after 36 weeks 36% vs 1% (controls); 20 fish with adenoma, 6 with hepatocellular carcinoma		Exposures carried out at 26°C in the dark; concentration exceeds saturation solubility of BaP	Hawkins et al, 1988; Hawkins et al., 1990
guppy, <i>Poecilia reticulata</i> (6-10 d old)	Water; dimethyl-formamide carrier.	Lab; static	BaP	209 µg/L	2 x 6h, 1 week apart	Neoplastic lesions in livers and other tissues after 52 weeks 23% vs 0% (controls); 1 altered foci, 5 adenoma, 4 with hepatocellular carcinoma		Studies carried out longer because tumorigenic response in guppy is slower than in medaka	Hawkins et al, 1988; Hawkins et al., 1990
Rainbow trout (fingerlings), <i>Oncorhynchus mykiss</i>	oral	Lab	BaP	1,000 ppm per feeding	12 and 18 months	Incidence of neoplasms on liver 15% (1.0/liver) at 12 months 25% (7.7/liver) at 18 months	-	MFO info also available 0% at 6 months 0% on other organs	Hendricks et al., 1985
Rainbow trout (juvenile), <i>Oncorhynchus mykiss</i> (10 mo)	ip injection	Lab	BaP	1 mg B(a)P in 0.4 ml PG (1/month for 12 months)	18 months (6 months after final injection)	Incidence of neoplasms in various organs = 46% (x = 7.7 tumors/organ)	-	Organs examined = gonads, swim bladder, liver, spleen, head and trunk kidneys, pancreas, intestines, and stomach	Hendricks et al., 1985

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
Pacific herring (embryos), <i>Clupea pallasii</i>	seawater contaminated by contact with oiled gravel - experiment 2; more weathered	lab; state	Field Mixture ^A	0.41 µ/L to 0.72 µ/L	16 days	- yolk sac edema - pericardial edema - skeletal, spinal, and craniofacial abnormalities - anaphase aberration	0.022 µg/g wet weight	Crude Oil characterized for PAHs only; concentrations of individual PAHs not given	

^A Artificially weathered Alaska North Slope crude oil.

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
Calif. grunion (embryos), <i>Leuresthes tenuis</i>	water	lab; static	BaP	measured: 5-24 µg/L (steady state); 24-361 µg/L (initial)	15 days	-retarded growth (14d) -sporadic heart beat -displaced head relative to yolk-sac -absence of melanophores near lateral lines -absence of lens formation -lesions as larvae (above)	day 15: 0.92 to 10.48 µg/g wet weight; 6.87 to 62.80 µg/g (dry weight)	-steady state concentration reached in 4 to 10 days	Winkler et al., 1983
Calif. grunion (embryos), <i>Leuresthes tenuis</i>	water	lab; static	BaP	measured: 869 ppb (initial); steady-state not reached	15 days	-retarded growth (14d) -lateral curvature mid-body -absent melanophores -unused yolk sac -lesions as larvae (above)	day 15 - 19.98 µg/g wet weight; 112.03 µg/g dry weight	steady-state concentration never reached	Winkler et al., 1983
Pacific herring (embryos), <i>Clupea pallasii</i>	seawater contaminated by contact with oiled gravel - experiment 1; less weathered	lab; static	Field Mixture^	9.1 µ/L	16 days	-yolk sac edema	13.7 µg/g wet weight	Crude Oil characterized for PAHs only; concentrations of individual PAHs not given	Carls et al., 1999

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
coho salmon, (24 h Post fertilization), <i>Oncorhynchus kisutch</i>	water; 0.5% DMSO	lab; static exposure then flow-through	BaP	25,000 µg/L	24 h	None	0.54 decreasing to 0.15 nmol/mg protien from 2 to 68 d post fertilization	Conc. of BaP in tissue are not converted because wet weights were not given; only the mg protein/animal. Can possibly borrow weights from earlier paper.	Ostrander et al., 1989
coho salmon, (32 d post fertilization), <i>Oncorhynchus kisutch</i>	water; 0.5% DMSO	lab; static exposure then flow-through	BaP	25,000 µg/L	24 h	None	4.47 decreasing to 0.33 nmol/mg protien from 2 to 68 d post fertilization	Conc. of BaP in tissue are not converted because wet weights were not given; only the mg protein/animal. Can possibly borrow weights from earlier paper.	Ostrander et al., 1989
Calif. grunion (embryos), <i>Leuresthes tenuis</i>	water	lab; static	BaP	measured: 5 µg/L (steady-state); 24 µg/L (initial)	15 days	-reduction in % hatch -lateral folding of tail -absence of caudal fin folds -hemorrhagic lesion or congested vasculature in caudal region	day 15: 0.992 ppm (wet weight); 6.872 ppm (dry weight)	-steady state concentration reached in 4 to 10 days	Winkler et al., 1983

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
gizzard shad, <i>Dorosoma cepedianum</i>	water and/or sediment ingestion	lab; static	BaP	1.02 µg/g sediment (initial); 0.63 µg/g sediment (mean of days 4, 8, and 15)	22 days	none	ligated fish: 0.010 µg/g wet weight (n=4) non-ligated: 0.012 µg/g wet weight (n=14)	-50 shad, 30 ligated; 20 non-ligated, in 500 L H ₂ O with 3.15 kg sediment -no sig. decline in sediment conc. after day 4 -all other tissue concs. BDL (n=26 ligated; n=6 non-ligated)	Kolok et al., 1996
estuarine clams, <i>Rangia cuneata</i>	water; acetone carrier	lab; static	BaP	30.5 µg/L	24 h	none	7.2 µg/g wet weight	-majority of BaP concentrated in the viscera (~75%) -n=5	Neff and Anderson, 1975
estuarine clams, <i>Rangia cuneata</i>	water; acetone carrier	lab; static	BaP	30.5 µg/L	24 h	none	5.7 µg/g wet weight	-majority of BaP concentrated in the viscera (~65%) -n=8	Neff and Anderson, 1975
coho salmon (24 h Post fertilization), <i>Oncorhynchus kisutch</i>	water; 0.5% DMSO	lab; static exposure then flow-through	BaP	25,000 µg/L	24 h	None	-	Effects on hatching, orientation, and foraging only.	Ostrander et al., 1988
coho salmon, (32 d post fertilization), <i>Oncorhynchus kisutch</i>	water; 0.5% DMSO	lab; static exposure then flow-through	BaP	25,000 µg/L	24 h	None	-	Effects on hatching, orientation, and foraging only.	Ostrander et al., 1988

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
Sand sole (embryos), <i>Psettiichthys melanostichus</i>	water; static	lab	BaP	0.1 µg/L measured; range (0.08 - 0.12)	through to yolk-sac absorption (7 -10 d)	-overgrowth of tissues -arrested development -twinning; Effects only after 48 h, i.e., during organogenesis	2.1 µg/g wet weight	effects only exhibited in 5% of animals; average hatching success of controls only 57% versus 28% BaP-treated	Hose et al., 1982
Flathead sole (embryos), <i>Hippoglossoides elassodon</i>	water; static	lab	BaP bound to bovine serum albumin	4.2 µg/L decreasing to <0.05 µg/L (DL)	through to yolk-sac absorption (7 -10 d)	-hatching success sig. decrease -nuclear pycnosis and general disruption of neural and ocular tissues	-	very low hatching success in controls and experimental; 5.5 and 11.5%, respectively	Hose et al., 1982
English sole (embryos), <i>Parophrys vetulus</i>	water	lab	BaP	2.1 µg/L measured	through to yolk-sac absorption (7 -10 d)	none	-	-	Hose et al., 1982
gizzard shad, <i>Dorosoma cepedianum</i>	water via treated sediment	lab; static	BaP	1.38 µg/g sediment (initial); 0.74 µg/g sediment (mean of days 4,8 and 15)	22 d	none	BDL in all but 2 fish on day 4 - (0.001 and 0.0002 µg/g wet weight)	-40 ligated shad in 250 L H ₂ O with 4.15 kg sediment -no sig. decline in sediment conc. after day 4.	Kolok et al., 1996

Appendix E. Teratogenic effects from laboratory exposure to PAHs.

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
fathead minnow (embryos), <i>Pimephales promelas</i>	maternal via water	lab; flow-through	Anthracene	6.66 µg/L 11.6 µg/L	6 wks 3 wks	-yolk-sac malformations -edema -eye deformities	8.8a µg/g (eggs)	Effects on embryos incubated with solar ultraviolet light radiation	Hall and Oris, 1991
freshwater topminnows, <i>Poeciliopsis monacha</i> <i>Poeciliopsis lucida</i>	water; acetone carrier	lab; static renewal	BaP	1,000 µg/L nominal; 1,250 µg/L was acutely lethal	24 h followed by 6 mo. of monitoring	-increased AHH and EROD activities	9.0 µg/g converted from 35.7 nmol/g wet wt.	Implied effect - increased AHH and EROD activity indicative of carcinogenic and teratogenic metabolites formed during metabolism of BaP by MFO-system	Goddard et al., 1987
English sole (embryos), <i>Parophrys vetulus</i>	maternal via oral	lab; wild-caught	BaP	8,000 µg/L (8 mg/kg force-fed)	-	-malformation of tail regions -insufficient yolk-sac -reduced fin-fold size -reduced hatching success	51.2 and 263 µg/g (eggs) - avg. = 157; Tissue conc. from 80 mg/kg i.p. maternal injection	-Eggs maintained 11 days until yolk-sac absorbed; static. -Incidence of effect 4 times greater than controls (Chai-square df=3.81)	Hose et al., 1981
Rainbow trout (embryos), <i>Oncorhynchus mykiss</i>	aqueous from BaP spiked to sediment	lab; static renewal (7-10d)	BaP	0.21 µg/L measured	through to 36 d post-hatch	-nuclear pycnosis -lack of body pigment -insufficient yolk-sac -abnormalities of eyes -increased mortality (at 2.40 µg/L in aqueous) -muscle necrosis -abnormal mitosis in eyes and brains	1.93 µg/g (eggs), 12.34 µg/g (alevins), from exposure to 2.40 µg/L BaP	Poor control survival (52% mortality)	Hannah et al., 1982; Hose et al., 1984

^E Spiked sediments from Suedel et al. (1993) were unlikely at equilibrium; i.e., organisms were tested after only 18 to 24 hours after spiking.

Common Name, Scientific Name	Chemical	Response	Median Response Conc. ^A ($\mu\text{g/goc}$)	$C_{OC,PAH,FCVI}$ ($\mu\text{g/goc}$)	Test- Specific ESGU _{FCVI} ^B (Unitless)	PAH- Specific SMAV ^C	GMAV ^D	References ^E
<i>Eohaustorius estuarius</i>								
Amphipod, <i>Eohaustorius estuarius</i>	acenaphthene	10 d LC50	1920	489	3.93	4.82	-	Swartz et al., 1991a
Amphipod, <i>Eohaustorius estuarius</i>	phenanthrene	10 d LC50	4210	593	7.10	-	-	Swartz et al., 1991a
Amphipod, <i>Eohaustorius estuarius</i>	phenanthrene	10 d LC50	3760	593	6.34	-	-	Swartz et al., 1991a
Amphipod, <i>Eohaustorius estuarius</i>	phenanthrene	10 d LC50	4060	593	6.85	6.75	-	Swartz et al., 1991a
Amphipod, <i>Eohaustorius estuarius</i>	fluoranthene	10 d LC50	3100	704	4.40	-	-	DeWitt et al., 1989
Amphipod, <i>Eohaustorius estuarius</i>	fluoranthene	10 d LC50	3930	704	5.59	-	-	DeWitt et al., 1989
Amphipod, <i>Eohaustorius estuarius</i>	fluoranthene	10 d LC50	3570	704	5.07	5.00	5.46	DeWitt et al., 1989
Midge, <i>Chironomus tentans</i>	fluoranthene	10 d LC50	1590	704	-	-	-	Suedel et al., 1993
Midge, <i>Chironomus tentans</i>	fluoranthene	10 d LC50	1740	704	-	-	-	Suedel et al., 1993
Midge, <i>Chironomus tentans</i>	fluoranthene	10 d LC50	682	704	-	-	-	Suedel et al., 1993
Amphipod, <i>Diporeia</i> sp.	pyrene	31 d LC50	>9090	694	>13.1	-	-	Landrum et al., 1994
Amphipod, <i>Diporeia</i> sp.	fluoranthene	10 d LC50	(147000) >23900 (29300)	704	>34.0	>34.0	>34.0	Driscoll et al., 1997a

^A Bolded median response concentration (acute) values are the $C_{OC,PAH,M_{sol}}$ based on the water solubilities of the PAH (Mackay et al., 1992). For these tests the interstitial water concentration at the median response concentration exceeded solubility. Therefore, solubilities are used instead of the acute value for further calculations.

^B Test-specific ESGUs: Quotient of the median response concentration ($\mu\text{g/goc}$) and $C_{OC,PAH,FCVI}$ (from Table 3-4).

^C PAH-specific SMAV: Geometric mean of the test-specific ESGTU_{FCVI} values from 10-d LC50 tests by species and PAH. Test-specific ESGTU_{FCVI} values greater than solubility included only if they are the sole 10-d LC50 for the species.

^D GMAV: Geometric mean of the PAH-specific SMAVs for all species within a genus.

Common Name, <i>Scientific Name</i>	Chemical	Response	Median Response Conc. ^A ($\mu\text{g/goc}$)	$C_{OC,PAH,FCVI}$ ($\mu\text{g/goc}$)	Test- Specific ESGU _{FCVI} ^B (Unitless)	PAH- Specific SMAV ^C	GMAV ^D	References ^E
Amphipod, <i>Rhepoxynius abronius</i>	pyrene	10 d LC50	2810	694	4.05	2.67	-	Swartz et al., 1997
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	> 4360	704	> 6.19	-	-	DeWitt et al., 1992
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	4410	704	6.26	-	-	DeWitt et al., 1992
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	3080	704	4.38	-	-	DeWitt et al., 1992
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	2230	704	3.17	-	-	Swartz et al., 1990
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	3150	704	4.50	-	-	DeWitt et al., 1992
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	1890	704	2.68	-	-	Swartz et al., 1990
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	2790	704	3.96	-	-	De Witt et al., 1992
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	2320	704	3.30	-	-	Swartz et al., 1997
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	1700	704	2.41	-	-	DeWitt et al., 1989
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	1030	704	1.47	-	-	Swartz et al., 1988
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	2100	704	2.98	-	-	Swartz et al., 1990
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	3310	704	4.70	3.56	3.67	Swartz et al., 1997
Amphipod, <i>Eohaustorius estuarius</i>	acenaphthene	10 d LC50	1630	489	3.33	-	-	Swartz et al., 1991a
Amphipod,	acenaphthene	10 d LC50	4180	489	8.55	-	-	Swartz et al., 1991a

Common Name, Scientific Name	Chemical	Response	Median Response Conc. ^A (µg/goc)	C _{OC,PAH,FCVI} (µg/goc)	Test- Specific ESGU _{FCVI} ^B (Unitless)	PAH- Specific SMAV ^C	GMAV ^D	References ^E
Amphipod, <i>Hyalella azteca</i>	fluoranthene	10 d LC50	5130	704	7.29	15.1	15.1	DeWitt et al., 1989
Amphipod, <i>Corophium spinicorne</i>	fluoranthene	10 d LC50	2830	704	4.02	-	-	Swartz et al., 1990
Amphipod, <i>Corophium spinicorne</i>	fluoranthene	10 d LC50	4390	704	6.23	5.01	5.01	Swartz et al., 1990
Amphipod, <i>Leptocheirus plumulosus</i>	acenaphthene	10 d LC50	10900	489	22.3	-	-	Swartz et al., 1991a
Amphipod, <i>Leptocheirus plumulosus</i>	acenaphthene	10 d LC50	23500	489	48.1	-	-	Swartz et al., 1991a
Amphipod, <i>Leptocheirus plumulosus</i>	acenaphthene	10 d LC50	8450	489	17.3	26.4	-	Swartz et al., 1991a
Amphipod, <i>Leptocheirus plumulosus</i>	phenanthrene	10 d LC50	6870	593	11.59	-	-	Swartz et al., 1991a
Amphipod, <i>Leptocheirus plumulosus</i>	phenanthrene	10 d LC50	8080	593	13.63	-	-	Swartz et al., 1991a
Amphipod, <i>Leptocheirus plumulosus</i>	phenanthrene	10 d LC50	8180	593	13.8	13.0	18.5	Swartz et al., 1991a
Amphipod, <i>Rhepoxynius abronius</i>	acenaphthene	10 d LC50	2310	489	4.72	-	-	Swartz et al., 1997
Amphipod, <i>Rhepoxynius abronius</i>	acenaphthene	10 d LC50	2110	489	4.31	4.51	-	Swartz et al., 1997
Amphipod, <i>Rhepoxynius abronius</i>	phenanthrene	10 d LC50	3080	593	5.19	-	-	Swartz et al., 1997
Amphipod, <i>Rhepoxynius abronius</i>	phenanthrene	10 d LC50	2220	593	3.74	4.41	-	Swartz et al., 1997
Amphipod, <i>Rhepoxynius abronius</i>	pyrene	10 d LC50	1220	694	1.76	-	-	Swartz et al., 1997

APPENDIX D. Comparison of PAH-specific equilibrium partitioning sediment guidelines (ESGs) derived from narcosis theory and the median response concentration of benthic species for individual PAHs in spiked-sediment toxicity tests.

Common Name, Scientific Name	Chemical	Response	Median Response Conc. ^a (µg/goc)	C _{OC,PAH,FCVI} (µg/goc)	Test- Specific ESGU _{FCVI} ^b (Unitless)	PAH- Specific SMAV ^c	GMAV ^d	References ^e
Oligochaete, <i>Lumbriculus variegatus</i>	pyrene	7 d LC50	> 9090 (61100)	694	> 13.1	-	-	Kukkonen and Landrum, 1994
Oligochaete, <i>Lumbriculus variegatus</i>	pyrene	7 d EC50-SA	> 9090 (51400)	694	> 13.1	-	-	Kukkonen and Landrum, 1994
Oligochaete, <i>Limnodrilus hoffmeisteri</i>	phenanthrene	10 d LC50	> 34300 (42500)	593	> 57.8	> 57.8	> 57.8	Lotufo and Fleeger, 1996
Oligochaete, <i>Limnodrilus hoffmeisteri</i>	phenanthrene	28 d EC25-R	5790	593	9.80	-	-	Lotufo and Fleeger, 1996
Oligochaete, <i>Limnodrilus hoffmeisteri</i>	pyrene	28 d EC25-R	8440	694	12.2	-	-	Lotufo and Fleeger, 1996
Cladoceran, <i>Daphnia magna</i>	fluoranthene	10 d LC50	2380	704	-	-	-	Suedel et al., 1993
Cladoceran, <i>Daphnia magna</i>	fluoranthene	10 d LC50	955	704	-	-	-	Suedel et al., 1993
Cladoceran, <i>Daphnia magna</i>	fluoranthene	10 d LC50	3260	704	-	-	-	Suedel et al., 1993
Amphipod, <i>Hyaella azteca</i>	fluoranthene	10 d LC50	> 23900 (37649)	704	-	-	-	Driscoll et al., 1997a
Amphipod, <i>Hyaella azteca</i>	fluoranthene	10 d LC50	1250	704	-	-	-	Suedel et al., 1993
Amphipod, <i>Hyaella azteca</i>	fluoranthene	10 d LC50	1480	704	-	-	-	Suedel et al., 1993
Amphipod, <i>Hyaella azteca</i>	fluoranthene	10 d LC50	500	704	-	-	-	Suedel et al., 1993
Amphipod, <i>Hyaella azteca</i>	fluoranthene	10 d LC50	22000	704	31.3	-	-	Harkey et al., 1997

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^A	HABITAT ^B	PAH TESTED (CAS #)	LOG K _{OW} ^C	METHOD ^D	CONCENTRATION ^E	LC50/EC50 ^F (μg/L)	LC50/EC50 ^F (μmol/L)	PAH SPECIFIC SMAV ^H (μmol/L)	K _{OW} NORMALIZED PAH SPECIFIC SMAV ^I (μmol/g _{OC})	SPECIES SMAV ^J (μmol/g _{OC})	GMAV ^K (μmol/g _{OC})	REFERENCES
Inland silverside, <i>Menidia beryllina</i>	X	W	acenaphthene (83-32-9)	4.01	S	U	2300	14.9	-	-	-	-	Horne et al., 1983
Inland silverside, <i>Menidia beryllina</i>	J	W	acenaphthene (83-32-9)	4.01	R	U	>3800 (5564)	>24.6	>19.2	>150	-	-	Thursby et al., 1989a
Inland silverside, <i>Menidia beryllina</i>	J	W	pyrene (192-00-0)	4.92	FT	M	>132 (>188.17)	>0.653	>0.653	>29.2	-	-	Champlin and Poucher, 1992c
Inland silverside, <i>Menidia beryllina</i>	J	W	fluoranthene (206-44-0)	5.08	S	U	>260 (>616)	>1.29	>1.29	>82.0	>65.8	-	Spehar et al., 1999
Atlantic silverside, <i>Menidia menidia</i>	A	W	phenanthrene (85-01-8)	4.57	FT	M	108	0.606	0.606	12.6	12.6	28.8	Battelle Ocean Sciences, 1987
Winter flounder,	J	-	fluoranthene (206-44-0)	5.08	S	M	>188	>0.929	>0.929	>59.2	>59.2	>59.2	Spehar et al., 1999

^ALife-stage: A = adult, J = juvenile, L = larvae, E = embryo, U = life-stage and habitat unknown, X = life-stage unknown but habitat known.

^BHabitat: I = infauna, E = epibenthic, W = water column.

^Clog K_{OW}: Predicted using SPARC (Karickhoff et al, 1991).

^DMethod: S = static, R = renewal, FT = flow-through.

^EConcentration: U = unmeasured (nominal), M = chemical measured.

^FAcute Values: 96 hour LC50 or EC50, except for *Daphnia* and *Tanytarsus* which are 48 hours duration.

^GBolded acute values are the water solubilities of the PAH (Mackay et al., 1992). For these tests the acute values exceeded solubility. Therefore, solubilities are used instead of the acute value for further calculations.

^HPAH-specific SMAV: Geometric mean of the acute values by PAH and species.

^IPAH-specific SMAVs at a log K_{OW} = 1.0; calculated as antilog (log₁₀LC50 + 0.945log₁₀K_{OW})/1000 (see Equation 2-33).

^JSpecies SMAV: Geometric mean of K_{OW}-normalized SMAVs for a species across PAHs.

^KGMAV: Geometric mean of SMAVs for all species within a genus.

^LNot used in calculations.

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^A	HABITAT ^B	PAH TESTED (CAS #)	LOG K _{ow} ^C	METHOD ^D	CONCENTRATION ^E	LC50/EC50 ^F (µg/L)	LC50/EC50 ^F (µmol/L)	PAH SPECIFIC SMAV ^H (µmol/L)	K _{ow} NORMALIZED PAH SPECIFIC SMAV ^I (µmol/g _{oc})	SPECIES SMAV ^J (µmol/g _{oc})	GMAV ^K (µmol/g _{oc})	REFERENCES
Pink salmon, <i>Oncorhynchus gorbuscha</i>	Fry	W	naphthalene (91-20-3)	3.36	FT	M	960	7.49	-	-	-	-	Rice and Thomas, 1989
Pink salmon, <i>Oncorhynchus gorbuscha</i>	Fry	W	naphthalene (91-20-3)	3.36	FT	M	900	7.02	-	-	-	-	Rice and Thomas, 1989
Pink salmon, <i>Oncorhynchus gorbuscha</i>	Fry	W	naphthalene (91-20-3)	3.36	FT	M	990	7.72	-	-	-	-	Rice and Thomas, 1989
Pink salmon, <i>Oncorhynchus gorbuscha</i>	Fry	W	naphthalene (91-20-3)	3.36	FT	M	1010	7.88	-	-	-	-	Rice and Thomas, 1989
Pink salmon, <i>Oncorhynchus gorbuscha</i>	Fry	W	naphthalene (91-20-3)	3.36	FT	M	890	6.94	7.40	11.0	11.0	11.0	Rice and Thomas, 1989
Sheepshead minnow, <i>Cyprinodon variegatus</i>	J	E,W	acenaphthene (83-32-9)	4.01	S	U	2200	14.3	-	-	-	-	Heitmuller et al., 1981
Sheepshead minnow, <i>Cyprinodon variegatus</i>	J	E,W	acenaphthene (83-32-9)	4.01	R	U	> 3800 (50000)	> 25	-	-	-	-	Thursby et al., 1989a
Sheepshead minnow, <i>Cyprinodon variegatus</i>	A	E,W	acenaphthene (83-32-9)	4.01	FT	M	3100	20.1	20.1	124	-	-	Ward et al., 1981
Sheepshead minnow, <i>Cyprinodon variegatus</i>	J	E,W	phenanthrene (85-01-8)	4.57	R	U	> 245	> 1.37	-	-	-	-	Battelle Ocean Sciences, 1987
Sheepshead minnow, <i>Cyprinodon variegatus</i>	J	E,W	phenanthrene (85-01-8)	4.57	FT	M	429.4	2.41	2.41	50.0	-	-	Battelle Ocean Sciences, 1987
Sheepshead minnow, <i>Cyprinodon variegatus</i>	J	E,W	pyrene (129-00-0)	4.92	FT	M	> 132 (> 640)	> 0.653	> 0.653	> 29.2	-	-	Champlin and Poucher, 1992b
Sheepshead minnow, <i>Cyprinodon variegatus</i>	J	E,W	fluoranthene (206-44-0)	5.08	S	U	> 260 (> 20000)	> 1.29	-	-	-	-	Champlin and Poucher, 1992a; Spehar et al., 1999
Sheepshead minnow, <i>Cyprinodon variegatus</i>	J	E,W	fluoranthene (206-44-0)	5.08	S	U	> 260 (> 560000)	> 1.29	> 1.29	> 82 ^L	78.7	78.7	Heitmuller et al., 1981; U.S EPA, 1978

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^A	HABITAT ^B	PAH TESTED (CAS #)	LOG K _{ow} ^C	METHOD ^D	CONCENTRATION ^E	LC50/EC50 ^H (μg/L)	LC50/EC50 ^I (μmol/L)	PAH SPECIFIC SMAV ^H (μmol/L)	K _{ow} NORMALIZED PAH SPECIFIC SMAV ^I (μmol/g _{oc})	SPECIES SMAV ^J (μmol/g _{oc})	GMAV ^K (μmol/g _{oc})	REFERENCES
<i>Enallagma suckleyi</i>			(91-20-3)										
Grass shrimp, <i>Palaemonetes pugio</i>	X	E,W	naphthalene (91-20-3)	3.36	S	M	2350	18.3	18.3	27.2	-	-	Tatem et al., 1978
Grass shrimp, <i>Palaemonetes pugio</i>	X	E,W	acenaphthene (83-32-9)	4.01	S	U	676.8	4.39	-	-	-	-	Horne et al., 1983; Thursby, 1991b
Grass shrimp, <i>Palaemonetes pugio</i>	L	E,W	acenaphthene (83-32-9)	4.01	R	U	1697	11.0	6.95	43.0	-	-	Thursby et al., 1989a
Grass shrimp, <i>Palaemonetes pugio</i>	A	E,W	phenanthrene (85-01-8)	4.57	R	U	200.8	1.127	-	-	-	-	Battelle Ocean Sciences, 1987
Grass shrimp, <i>Palaemonetes pugio</i>	A	E,W	phenanthrene (85-01-8)	4.57	FT	M	145.4	0.816	0.816	17.0	-	-	Battelle Ocean Sciences, 1987
Grass shrimp, <i>Palaemonetes pugio</i>	J	E,W	fluoranthene (206-44-0)	5.08	S	U	142	0.702	0.702	44.7	30.7	30.7	Spehar et al., 1999
Sand shrimp, <i>Crangon septemspinosus</i>	X	E	acenaphthene (83-32-9)	4.01	S	U	245	1.59	1.59	4.80	9.80	9.80	Horne et al., 1983; Thursby, 1991b
American Lobster, <i>Homarus americanus</i>	L	-	fluoranthene (206-44-0)	5.08	R	U	>260 (317)	1.29	1.29	81.9	81.9	81.9	Spehar et al., 1999
Hermit crab, <i>Paquetus longicarpus</i>	A	E	phenanthrene (85-01-8)	4.57	FT	M	163.7	0.918	0.918	19.2	19.2	19.2	Battelle Ocean Sciences, 1987
Slipper limpet, <i>Crepidula fornicata</i>	L	W	acenaphthene (83-32-9)	4.01	R	U	3436	22.3	22.3	138	138	138	Thursby et al., 1989a
Sea urchin, <i>Arbacia punctulata</i>	E	W	acenaphthene (83-32-9)	4.01	S	U	>3800 (8163)	>24.6	>24.6	>152	-	-	Thursby et al., 1989a
Sea urchin, <i>Arbacia punctulata</i>	E	W	fluoranthene (206-44-0)	5.08	S	U	>260 (20000)	>1.3	>1.3	>82	>117	>117	Spehar et al., 1999

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^A	HABITAT ^B	PAH TESTED (CAS #)	LOG K _{ow} ^C	METHOD ^D	CONCENTRATION ^E	LC50/EC50 ^F (μg/L)	LC50/EC50 ^F (μmol/L)	PAH SPECIFIC SMAV ^H (μmol/L)	K _{ow} NORMALIZED PAH SPECIFIC SMAV ^I (μmol/g _{oc})	SPECIES SMAV ^J (μmol/g _{oc})	GMAV ^K (μmol/g _{oc})	REFERENCES
Isopod <i>Excirrolana vancouverensis</i>	J	I,E	fluoranthene (206-44-0)	5.08	R	M	>70	>0.346	>0.346	>22.1	>22.1	>22.1	Boese et al., 1997
Amphipod, <i>Ampelisca abdita</i>	J	I	acenaphthene (83-32-9)	4.01	R	U	1125	7.30	7.30	45.1	-	-	Thursby et al., 1989a
Amphipod, <i>Ampelisca abdita</i>	J	I	fluoranthene (206-44-0)	5.08	S	U	67	0.33	0.33	21.1	30.8	30.8	Spehar et al., 1999
Amphipod, <i>Leptocheirus plumulosus</i>	A	E,I	acenaphthene (83-32-9)	4.01	FT	M	589.4	3.82	3.82	23.6	-	-	Swartz, 1991a
Amphipod, <i>Leptocheirus plumulosus</i>	A	E,I	phenanthrene (85-01-8)	4.57	FT	M	198.4	1.11	1.11	23.2	-	-	Swartz, 1991a
Amphipod, <i>Leptocheirus plumulosus</i>	J	E,I	pyrene (129-00-0)	4.92	FT	M	66.49	0.329	0.329	14.7	-	-	Champlin and Poucher, 1992c
Amphipod, <i>Leptocheirus plumulosus</i>	X	E,I	fluoranthene (206-44-0)	5.08	R	M	51	0.252	0.252	16.1	19.0	19.0	Boese et al., 1997
Amphipod, <i>Rhepoxynius abronius</i>	J	I	fluoranthene (206-44-0)	5.08	R	M	63	0.311	0.311	19.9	19.9	19.9	Boese et al., 1997
Amphipod, <i>Eohaustorius estuarius</i>	J	I	fluoranthene (206-44-0)	5.08	R	M	>70	>0.346	>0.346	>22.1	>22.1	>22.1	Boese et al., 1997
Amphipod, <i>Grandidierella japonica</i>	J	I	fluoranthene (206-44-0)	5.08	R	M	27	0.133	0.133	8.5	8.5	8.5	Boese et al., 1997
Amphipod, <i>Corophium insidiosum</i>	J	I	fluoranthene (206-44-0)	5.08	R	M	54	0.267	0.267	17.0	17.0	17.0	Boese et al., 1997
Amphipod, <i>Emerita analoga</i>	J	I,E	fluoranthene (206-44-0)	5.08	R	M	74	0.366	0.366	23.3	23.3	23.3	Boese et al., 1997
Kelp shrimp	X	W	naphthalene	3.36	FT	M	1390	10.8	10.8	16.1	16.1	16.1	Rice and Thomas, 1989

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^A	HABITAT ^B	PAH TESTED (CAS #)	LOG K _{OW} ^C	METHOD ^D	CONCENTRATION ^E	LC50/EC50 ^F (μg/L)	LC50/EC50 ^F (μmol/L)	PAH SPECIFIC SMAV ^H (μmol/L)	K _{OW} NORMALIZED		SPECIES SMAV ^I (μmol/g _{OC})	GMAV ^K (μmol/g _{OC})	REFERENCES
										PAH SPECIFIC	PAH SPECIFIC			
Mysid, <i>Americamysis bahia</i>	J	E	acenaphthene (83-32-9)	4.01	FT	M	460	2.98	-	-	-	-	-	Thursby et al., 1989b
Mysid, <i>Americamysis bahia</i>	J	E	acenaphthene (83-32-9)	4.01	FT	M	190	1.23	-	-	-	-	-	EG&G Bionomics, 1982
Mysid, <i>Americamysis bahia</i>	J	E	acenaphthene (83-32-9)	4.01	FT	M	466.1	3.02	-	-	-	-	-	Horne et al., 1983; Thursby, 1991a
Mysid, <i>Americamysis bahia</i>	J	E	acenaphthene (83-32-9)	4.01	FT	M	271.9	1.76	2.10	13.0	-	-	-	Horne et al., 1983; Thursby, 1991a
Mysid, <i>Americamysis bahia</i>	J	E	phenanthrene (85-01-8)	4.57	FT	M	27.1	0.152	-	-	-	-	-	Kuhn and Lussier, 1987
Mysid, <i>Americamysis bahia</i>	J	E	phenanthrene (85-01-8)	4.57	FT	M	17.7	0.099	0.123	2.60	-	-	-	Battelle Ocean Sciences, 1987
Mysid, <i>Americamysis bahia</i>	J	E	pyrene (129-00-0)	4.92	FT	M	28.28	0.140	0.140	6.30	-	-	-	Champlin and Poucher, 1992c
Mysid, <i>Americamysis bahia</i>	J	E	fluoranthene (206-44-0)	5.08	S	U	31	0.153	-	-	-	-	-	Spehar et al., 1999
Mysid, <i>Americamysis bahia</i>	J	E	fluoranthene (206-44-0)	5.08	S	U	40	0.198	-	-	-	-	-	U.S. EPA, 1978
Mysid, <i>Americamysis bahia</i>	J	E	fluoranthene (206-44-0)	5.08	FT	M	30.53	0.151	-	-	-	-	-	Champlin and Poucher, 1992b; Spehar et al., 1999
Mysid, <i>Americamysis bahia</i>	J	E	fluoranthene (206-44-0)	5.08	FT	M	87	0.430	0.255	16.2	7.66	7.66	-	EG&G Bionomics, 1978
Mysid, <i>Neomysis americana</i>	X	E	naphthalene (91-20-3)	3.36	S	M	1250	9.75	-	-	-	-	-	Hargreaves et al., 1982
Mysid, <i>Neomysis americana</i>	X	E	naphthalene (91-20-3)	3.36	S	M	1420	11.1	10.4	15.4	15.4	15.4	-	Hargreaves et al., 1982

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^A	HABITAT ^B	PAH TESTED (CAS #)	LOG K _{ow} ^C	METHOD ^D	CONCENTRATION ^E	LC50/EC50 ^F (μg/L)	LC50/EC50 ^F (μmol/L)	PAH SPECIFIC SMAV ^H	K _{ow} NORMALIZED PAH SPECIFIC SMAV ^I	SPECIES SMAV ^I	GMAV ^K	REFERENCES
									(μmol/L)	(μmol/g _{oc})	(μmol/g _{oc})	(μmol/g _{oc})	
Blue mussel, <i>Mytilus edulis</i>	A	E,W	phenanthrene (85-01-8)	4.57	R	M	>245	>1.37	>1.37	>28.7	>28.7	>28.7	Battelle Ocean Sciences, 1987
Pacific oyster, <i>Crassostrea gigas</i>	E/L	W	naphthalene (91-20-3)	3.36	S	U	>31000 (199000)	>242	>242	>359	>359	>359	U.S. EPA, 1980
Coot clam, <i>Mulinia lateralis</i>	J	E	pyrene (129-00-0)	4.92	FT	M	>132 (>240)	>0.653	>0.653	>29.2	-	-	Champlin and Poucher, 1992c
Coot clam, <i>Mulinia lateralis</i>	J	E	fluoranthene (206-44-0)	5.08	S	U	>260 (10710)	>1.29	>1.29	>82.0	>48.9	>48.9	Spehar et al., 1999
Soft-shell clam, <i>Mya arenaria</i>	A	I	phenanthrene (85-01-8)	4.57	R	M	>245	>1.37	>1.37	>28.7	>28.7	>28.7	Battelle Ocean Sciences, 1987
Calanoid copepod <i>Eurytemora affinis</i>	A	X	naphthalene (91-20-3)	3.36	S	U	3798	22.6	22.6	33.5	-	-	Ott, et al., 1978
Calanoid copepod <i>Eurytemora affinis</i>	A	X	2-methyl naphthalene (91-57-6)	3.86	S	U	1499	7.74	7.74	34.2	-	-	Ott, et al., 1978
Calanoid copepod <i>Eurytemora affinis</i>	A	X	2,6-dimethyl naphthalene (581-42-0)	4.37	S	M	852	3.9	3.9	52.0	-	-	Ott, et al., 1978
Calanoid copepod <i>Eurytemora affinis</i>	A	X	2,3,5-trimethyl naphthalene (2245-38-7)	4.86	S	M	316	1.3	1.3	50.0	41.5	41.5	Ott, et al., 1978
Mysid, <i>Americamysis bahia</i>	J	E	acenaphthene (83-32-9)	4.01	S	U	970	6.29	-	-	-	-	U.S. EPA, 1978; Ward et al., 1981
Mysid, <i>Americamysis bahia</i>	J	E	acenaphthene (83-32-9)	4.01	S	M	160	1.04	-	-	-	-	EG&G Bionomics, 1982
Mysid, <i>Americamysis bahia</i>	J	E	acenaphthene (83-32-9)	4.01	R	U	1190	7.72	-	-	-	-	Thursby et al., 1989a

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Bluegill, <i>Lepomis macrochirus</i>	J	W	fluoranthene (206-44-0)	5.08	S	U	>260 (4000)	>1.3	-	-	-	-	Buccafusco et al., 1981; EPA, 1978
Bluegill, <i>Lepomis macrochirus</i>	J	W	fluoranthene (206-44-0)	5.08	FT	M	44	0.218	0.218	13.9	34.0	34.0	Spehar et al., 1999
South african clawed frog <i>Xenopus laevis</i>	L	W	naphthalene (91-20-3)	3.36	FT	M	2100	16.38	-	-	-	-	Edmisten and Bantle, 1982
South african clawed frog <i>Xenopus laevis</i>	L	W	naphthalene (91-20-3)	3.36	FT	M	2100	16.38	16.38	24.3	24.3	24.3	Edmisten and Bantle, 1982
<u>SALTWATER</u>													
Annelid worm, <i>Neanthes arenaceodentata</i>	J	I	naphthalene (91-20-3)	3.36	S	U	3800	29.6	29.6	44.0	-	-	Rossi and Neff, 1978
Annelid worm, <i>Neanthes arenaceodentata</i>	X	I	acenaphthene (83-32-9)	4.01	S	U	3600	23.3	-	-	-	-	Horne et al., 1983
Annelid worm, <i>Neanthes arenaceodentata</i>	J	I	acenaphthene (83-32-9)	4.01	R	U	>3800 (16440)	>24.6	23.3	144	-	-	Thursby et al., 1989a
Annelid worm, <i>Neanthes arenaceodentata</i>	A	I	phenanthrene (85-01-8)	4.57	S	U	600	3.37	3.37	70.0	-	-	Rossi and Neff, 1978
Annelid worm, <i>Neanthes arenaceodentata</i>	J	I	fluoranthene (206-44-0)	5.08	S	U	>260 (500)	>1.29	-	-	-	-	Rossi and Neff, 1978
Annelid worm, <i>Neanthes arenaceodentata</i>	J	I	fluoranthene (206-44-0)	5.08	S	U	>260 (20000)	>1.29	>1.29	>82 ^l	76.3	76.3	Spehar et al., 1999
Archiannelid, <i>Dinophilus gyrociliatus</i>	J	I	phenanthrene (85-01-8)	4.57	R	U	185.40	1.04	1.04	21.7	21.7	21.7	Battelle Ocean Sciences, 1987
Mud snail, <i>Nassarius obsoletus</i>	A	I,E	phenanthrene (85-01-8)	4.57	R	M	>245	>1.37	>1.37	>28.7	>28.7	>28.7	Battelle Ocean Sciences, 1987

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^A	HABITAT ^B	PAH TESTED (CAS #)	LOG K _{ow} ^C	METHOD ^D	CONCENTRATION ^E	LC50/EC50 ^H (μg/L)	LC50/EC50 ^F (μmol/L)	PAH SPECIFIC SMAV ^H (μmol/L)	K _{ow} NORMALIZED PAH SPECIFIC SMAV ^I (μmol/g _{oc})	SPECIES SMAV ^I (μmol/g _{oc})	GMAV ^K (μmol/g _{oc})	REFERENCES
<i>Pimephales promelas</i>			(83-32-9)										
Fathead minnow, <i>Pimephales promelas</i>	J	W	acenaphthene (83-32-9)	4.01	FT	M	1600	10	7.71	48.0	-	-	Holcombe et al., 1983
Fathead minnow, <i>Pimephales promelas</i>	X	W	fluorene (86-73-7)	4.21	S	U	> 1900 (100000)	> 11.4	> 11.4	> 108 ^L	-	-	Finger et al., 1985
Fathead minnow, <i>Pimephales promelas</i>	J	W	phenanthrene (85-01-8)	4.57	S	M	> 1100 (> 1150)	> 6.17	> 6.17	> 129 ^L	-	-	U.S. EPA, 1978
Fathead minnow, <i>Pimephales promelas</i>	J	W	fluoranthene (206-44-0)	5.08	S	M	95	0.470	-	-	-	-	Horne and Oblad, 1983
Fathead minnow, <i>Pimephales promelas</i>	J	W	fluoranthene (206-44-0)	5.08	S	M	7.71	0.0381	-	-	-	-	Gendusa, 1990
Fathead minnow, <i>Pimephales promelas</i>	A	W	fluoranthene (206-44-0)	5.08	FT	U	> 260 (> 1000)	> 1.29	-	-	-	-	Birge et al., 1982
Fathead minnow, <i>Pimephales promelas</i>	J	W	fluoranthene (206-44-0)	5.08	FT	M	69	0.34	0.34	22.0	68.3	68.3	Spehar et al., 1999
Channel catfish, <i>Ictalurus punctatus</i>	J	E	acenaphthene (83-32-9)	4.01	FT	M	1720	11.2	11.2	69.0	-	-	Holcombe et al., 1983
Channel catfish, <i>Ictalurus punctatus</i>	J	E	fluoranthene (206-44-0)	5.08	S	M	37.40	0.185	0.185	12.0	28.8	28.8	Gendusa, 1990
Bluegill, <i>Lepomis macrochirus</i>	J	W	acenaphthene (83-32-9)	4.01	S	U	1700	11.0	11.0	68	-	-	Buccafusco et al., 1981
Bluegill, <i>Lepomis macrochirus</i>	X	W	fluorene (86-73-7)	4.21	S	U	910	5.47	5.47	51.8	-	-	Finger et al., 1985
Bluegill, <i>Lepomis macrochirus</i>	J	W	phenanthrene (85-01-8)	4.57	FT	M	234	1.31	1.31	27.4	-	-	Call et al., 1986

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Fathead minnow, <i>Pimephales promelas</i>	J	W	naphthalene (91-20-3)	3.36	S	M	1990	15.5	-	-	-	-	Millemann et al., 1984
Fathead minnow, <i>Pimephales promelas</i>	J	W	naphthalene (91-20-3)	3.36	FT	M	7900	61.6	-	-	-	-	DeGraeve et al., 1982
Fathead minnow, <i>Pimephales promelas</i>	X	W	naphthalene (91-20-3)	3.36	FT	M	4900	38.2	-	-	-	-	DeGraeve et al., 1980
Fathead minnow, <i>Pimephales promelas</i>	J	W	naphthalene (91-20-3)	3.36	FT	M	6140	47.9	-	-	-	-	Geiger et al., 1985
Fathead minnow, <i>Pimephales promelas</i>	J	W	naphthalene (91-20-3)	3.36	FT	M	8900	69.4	-	-	-	-	DeGraeve et al., 1980
Fathead minnow, <i>Pimephales promelas</i>	J	W	naphthalene (91-20-3)	3.36	FT	M	6080	47.4	51.8	76.8	-	-	Holcombe et al., 1984
Fathead minnow, <i>Pimephales promelas</i>	J	W	1-methyl naphthalene (90-12-0)	3.84	S	U	9000	63.4	63.4	268	-	-	Mattson et al., 1976
Fathead minnow, <i>Pimephales promelas</i>	J	W	acenaphthene (83-32-9)	4.01	S	M	3100	20	-	-	-	-	Marine Bioassay Lab., 1981
Fathead minnow, <i>Pimephales promelas</i>	J	W	acenaphthene (83-32-9)	4.01	S	M	1500	9.7	-	-	-	-	EG&G Bionomics, 1982
Fathead minnow, <i>Pimephales promelas</i>	A	W	acenaphthene (83-32-9)	4.01	R	U	3700	24	-	-	-	-	Academy of Natural Sci., 1981
Fathead minnow, <i>Pimephales promelas</i>	J	W	acenaphthene (83-32-9)	4.01	FT	M	1730	11.2	-	-	-	-	Geiger et al., 1985
Fathead minnow, <i>Pimephales promelas</i>	J	W	acenaphthene (83-32-9)	4.01	FT	M	608	3.94	-	-	-	-	Cairns and Nebeker, 1982
Fathead minnow, <i>Pimephales promelas</i>	J	W	acenaphthene	4.01	FT	M	>1400	>9.1	-	-	-	-	EG&G Bionomics, 1982

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									SMAV ^H (μmol/L)	PAH SPECIFIC SMAV ^I (μmol/g _{oc})	SMAV ^J (μmol/g _{oc})	(μmol/g _{oc})	
Rainbow trout <i>Oncorhynchus mykiss</i>	pre SU	I	naphthalene (91-20-3)	3.36	S	U	2600	20.3	-	-	-	-	Edsall, C.C., 1991
Rainbow trout <i>O. corhynchus mykiss</i>	pre SU	I	naphthalene (91-20-3)	3.36	S	U	4400	34.3	-	-	-	-	Edsall, C.C., 1991
Rainbow trout <i>Oncorhynchus mykiss</i>	pre SU	I	naphthalene (91-20-3)	3.36	S	U	5500	42.9	-	-	-	-	Edsall, C.C., 1991
Rainbow trout <i>Oncorhynchus mykiss</i>	J	W	naphthalene (91-20-3)	3.36	FT	M	1600	12.5	-	-	-	-	DeGraeve et al., 1982
Rainbow trout <i>Oncorhynchus mykiss</i>	X	W	naphthalene (91-20-3)	3.36	FT	M	2300	17.9	15.0	22.2	-	-	DeGraeve et al., 1980
Rainbow trout <i>Oncorhynchus mykiss</i>	J	W	acenaphthene (83-32-9)	4.01	FT	M	670	4.34	4.34	26.9	-	-	Holcombe et al., 1983
Rainbow trout <i>Oncorhynchus mykiss</i>	J	W	fluorene (86-73-7)	4.21	S	U	820	4.93	4.93	46.7	-	-	Finger et al., 1985
Rainbow trout <i>Oncorhynchus mykiss</i>	pre SU	I	1,3-dimethyl naphthalene (575-41-7)	4.37	S	U	1700	10.9	14.0	188 ^L	-	-	Edsall, C.C., 1991
Rainbow trout <i>Oncorhynchus mykiss</i>	L	W	phenanthrene (85-01-8)	4.57	S	U	> 1100 (3200)	> 6.2	-	-	-	-	Edsall, C.C., 1991
Rainbow trout <i>Oncorhynchus mykiss</i>	J	W	phenanthrene (85-01-8)	4.57	FT	M	375	2.10	2.10	43.9	-	-	Call et al., 1986
Rainbow trout <i>Oncorhynchus mykiss</i>	X	W	fluoranthene (206-44-0)	5.08	S	M	187	0.925	-	-	-	-	Horne and Oblad, 1983
Rainbow trout <i>Oncorhynchus mykiss</i>	J	W	fluoranthene (206-44-0)	5.08	FT	M	26.0	0.129	0.129	8.19	25.1	40.4	Spehar et al., 1999
Brown trout, <i>Salmo trutta</i>	J	W	acenaphthene (83-32-9)	4.01	FT	M	580	3.76	3.76	23.3	23.3	23.3	Holcombe et al., 1983

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Stonefly, <i>Peltopleria maria</i>	X	E	fluoranthene (206-44-0)	5.08	S	U	135	0.667	0.667	42.5	20.2	20.2	Horne and Oblad, 1983
Midge, <i>Chironomus tentans</i>	L	I	naphthalene (91-20-3)	3.36	S	M	2810	21.9	21.9	32.5	-	-	Millemann et al., 1984
Midge, <i>Chironomus tentans</i>	L	I	phenanthrene (85-01-8)	4.57	S	M	490	2.75	2.75	57.0	-	-	Millemann et al., 1984
Midge, <i>Chironomus tentans</i>	L	I	fluoranthene (206-44-0)	5.08	S	M	>250	>1.24	>1.24	>79 ^L	43.0	-	Suedel and Rodgers, 1996
Midge, <i>Chironomus riparius</i>	L	I	fluorene (86-73-7)	4.21	S	U	>1900 (2350)	>11.42	>11.42	>108	>108	>68.2	Finger et al., 1985
Midge, <i>Paratanytarsus sp.</i>	X	E	acenaphthene (83-32-9)	4.01	S	M	2000	13.0	-	-	-	-	Northwestern Aquatic Science Inc., 1982
Midge, <i>Paratanytarsus sp.</i>	X	E	acenaphthene (83-32-9)	4.01	S	M	2090	13.6	13.3	82	82	82	Northwestern Aquatic Science Inc., 1982
Midge <i>Tanytarsus dissimilis</i>	L	I	naphthalene (91-20-3)	3.36	S	U	20700	162	-	-	-	-	Darville and Wilhm, 1984
Midge <i>Tanytarsus dissimilis</i>	L	I	naphthalene (91-20-3)	3.36	S	U	12600	98.31	126	187	187	187	Darville and Wilhm, 1984
Coho salmon <i>Oncorhynchus kisutch</i>	E	I	naphthalene (91-20-3)	3.36	R	M	>11800	>92.1	-	-	-	-	Korn and Rice, 1981
Coho salmon <i>Oncorhynchus kisutch</i>	F	W	naphthalene (91-20-3)	3.36	R	M	5600	43.7	43.7	65.0	65.0	-	Korn and Rice, 1981
Rainbow trout <i>Oncorhynchus mykiss</i>	pre SU	I	naphthalene (91-20-3)	3.36	S	U	1800	14.0	-	-	-	-	Edsall, C.C., 1991
Rainbow trout <i>Oncorhynchus mykiss</i>	pre SU	I	naphthalene (91-20-3)	3.36	S	U	6100	47.6	-	-	-	-	Edsall, C.C., 1991

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Cladoceran, <i>Daphnia pulex</i>	X	W	phenanthrene (85-01-8)	4.57	S	U	>1100 (>1150)	>6.17	-	-	-	-	Geiger and Buikema, 1981, 1982
Cladoceran, <i>Daphnia pulex</i>	X	W	phenanthrene (85-01-8)	4.57	S	U	350	1.96	-	-	-	-	Smith et al., 1988
Cladoceran, <i>Daphnia pulex</i>	X	W	phenanthrene (85-01-8)	4.57	S	M	100	0.56	1.66	34.6	-	-	Trucco et al., 1983
Cladoceran, <i>Daphnia pulex</i>	X	W	2-methyl anthracene (613-12-7)	4.99	S	U	>30 (96)	>0.156	>0.156	>8.1 ^L	30.2	27.6	Smith et al., 1988
Amphipod, <i>Gammarus minus</i>	X	E	acenaphthene (83-32-9)	4.01	S	U	460	3.0	3.0	18.4	-	-	Horne et al., 1983
Amphipod, <i>Gammarus minus</i>	A	E	fluoranthene (206-44-0)	5.08	S	U	32	0.16	0.16	10.1	13.6	-	Horne and Oblad, 1983
Amphipod, <i>Gammarus pseudolimnaeus</i>	X	E	fluorene (86-73-7)	4.21	S	U	600	3.61	3.61	34.2	-	-	Finger et al., 1985
Amphipod, <i>Gammarus pseudolimnaeus</i>	X	E	phenanthrene (85-01-8)	4.57	FT	M	126	0.707	0.707	14.8	-	-	Call et al., 1986
Amphipod, <i>Gammarus pseudolimnaeus</i>	A	E	fluoranthene (206-44-0)	5.08	FT	M	43	0.213	0.213	13.5	19.0	16.1	Spehar et al., 1999
Amphipod, <i>Hyaella azteca</i>	J	E	fluoranthene (206-44-0)	5.08	FT	M	44	0.218	0.218	13.9	13.9	13.9	Spehar et al., 1999
Dragonfly, <i>Ophiogomphus</i> sp.	N	E	fluoranthene (206-44-0)	5.08	FT	M	>178	>0.880	>0.880	>56	>56	>56	Spehar et al., 1999
Stonefly, <i>Pelioperla maria</i>	X	E	acenaphthene (83-32-9)	4.01	S	U	240	1.6	1.6	9.6	-	-	Horne et al., 1983

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									SMAV ^H (μmol/L)	PAH SPECIFIC SMAV ^I (μmol/g _{oc})	PAH SPECIFIC SMAV ^I (μmol/g _{oc})	SMAV ^J (μmol/g _{oc})		
Cladoceran, <i>Daphnia magna</i>	J	W	pyrene (129-00-0)	4.92	S	U	90.9	0.45	0.45	20.1	-	-	-	Abernethy et al., 1986
Cladoceran, <i>Daphnia magna</i>	J	W	9-methyl anthracene (779-02-2)	5.01	S	U	124.8	0.65	0.65	34.9	-	-	-	Abernethy et al., 1986
Cladoceran, <i>Daphnia magna</i>	J	W	fluoranthene (206-44-0)	5.08	S	U	>260 (320000)	>1.29	-	-	-	-	-	LeBlanc, 1980a
Cladoceran, <i>Daphnia magna</i>	J	W	fluoranthene (206-44-0)	5.08	S	M	45	0.222	-	-	-	-	-	Oris et al., 1991
Cladoceran, <i>Daphnia magna</i>	J	W	fluoranthene (206-44-0)	5.08	R	M	117	0.578	-	-	-	-	-	Spehar et al., 1999
Cladoceran, <i>Daphnia magna</i>	X	W	fluoranthene (206-44-0)	5.08	S	M	105.7	0.523	0.407	25.9	25.2	-	-	Suedel and Rodgers, 1996
Cladoceran, <i>Daphnia pulex</i>	X	W	naphthalene (91-20-3)	3.36	S	U	4663	36.4	36.4	54.0	-	-	-	Smith et al., 1988
Cladoceran, <i>Daphnia pulex</i>	X	W	fluorene (86-73-7)	4.21	S	U	212	1.27	1.27	12.1	-	-	-	Smith et al., 1988
Cladoceran, <i>Daphnia pulex</i>	X	W	1,3-dimethyl naphthalene (575-41-7)	4.37	S	U	767	4.92	4.92	66	-	-	-	Smith et al., 1988
Cladoceran, <i>Daphnia pulex</i>	X	W	2,6-dimethyl naphthalene (581-42-0)	4.37	S	U	193	1.24	1.24	16.8	-	-	-	Smith et al., 1988
Cladoceran, <i>Daphnia pulex</i>	X	W	anthracene (120-12-7)	4.53	S	U	>45 (754)	>0.25	>0.25	>4.9 ^L	-	-	-	Smith et al., 1988
Cladoceran, <i>Daphnia pulex</i>	Neonate	W	phenanthrene (85-01-8)	4.57	S	U	734	4.12	-	-	-	-	-	Passino and Smith, 1987

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^A	HABITAT ^B	PAH TESTED (CAS #)	LOG K _{ow} ^C	METHOD ^D	CONCENTRATION ^E	LC50/EC50 ^F (μg/L)	LC50/EC50 ^F (μmol/L)	PAH SPECIFIC SMAV ^H (μmol/L)	K _{ow} NORMALIZED		SPECIES SMAV ^I (μmol/g _{oc})	GMAV ^K (μmol/g _{oc})	REFERENCES
										PAH SPECIFIC SMAV ^I	PAH SPECIFIC SMAV ^I			
Cladoceran, <i>Daphnia magna</i>	J	W	2-methyl naphthalene (91-57-6)	3.86	S	U	1491	10.5	10.5	46.3		-	-	Abernethy et al., 1986
Cladoceran, <i>Daphnia magna</i>	X	W	acenaphthene (83-32-9)	4.01	S	U	3450	22.4	-	-		-	-	Randall and Knopp, 1980
Cladoceran, <i>Daphnia magna</i>	X	W	acenaphthene (83-32-9)	4.01	S	U	> 3800 (41000)	> 24.6	-	-		-	-	LeBlanc, 1980a
Cladoceran, <i>Daphnia magna</i>	X	W	acenaphthene (83-32-9)	4.01	S	M	320	2.08	-	-		-	-	EG&G Bionomics, 1982
Cladoceran, <i>Daphnia magna</i>	X	W	acenaphthene (83-32-9)	4.01	S	M	1300	8.43	-	-		-	-	EG&G Bionomics, 1982
Cladoceran, <i>Daphnia magna</i>	X	W	acenaphthene (83-32-9)	4.01	FT	M	120	0.778	0.778	4.80		-	-	EG&G Bionomics, 1982
Cladoceran, <i>Daphnia magna</i>	X	W	fluorene (86-73-7)	4.21	S	U	430	2.59	2.59	24.5		-	-	Finger et al., 1985
Cladoceran, <i>Daphnia magna</i>	J	W	phenanthrene (85-01-8)	4.57	S	U	207	1.16	-	-		-	-	Abernethy et al., 1986
Cladoceran, <i>Daphnia magna</i>	X	W	phenanthrene (85-01-8)	4.57	S	U	843	4.73	-	-		-	-	Eastmond et al., 1984
Cladoceran, <i>Daphnia magna</i>	Neonate	W	phenanthrene (85-01-8)	4.57	S	M	700	3.93	-	-		-	-	Millemann et al., 1984
Cladoceran, <i>Daphnia magna</i>	Neonate	W	phenanthrene (85-01-8)	4.57	S,R	M	212	1.19	-	-		-	-	Brooke, 1994
Cladoceran, <i>Daphnia magna</i>	Neonate	W	phenanthrene (85-01-8)	4.57	FT	M	230	1.29	-	-		-	-	Brooke, 1993
Cladoceran, <i>Daphnia magna</i>	X	W	phenanthrene (85-01-8)	4.57	FT	M	117	0.656	0.920	19.2		-	-	Call et al., 1986

Appendix C. Summary of data on the acute toxicity of PAHs to freshwater and saltwater species and the derivation of genus mean acute values.

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^a	HABITAT ^b	PAH TESTED (CAS #)	LOG K _{ow} ^c	METHOD ^d	CONCENTRATION ^e	LC50/EC50 ^f (μg/L)	LC50/EC50 ^f (μmol/L)	PAH SPECIFIC SMAV ^h (μmol/L)	K _{ow} NORMALIZED PAH SPECIFIC SMAV ⁱ (μmol/g _{oc})	SPECIES SMAV ^j (μmol/g _{oc})	GMAV ^k (μmol/g _{oc})	REFERENCES
FRESHWATER													
Hydra, <i>Hydra americana</i>	J	W,E	fluoranthene (206-44-0)	5.08	FT	M	70	0.346	0.346	22.1	22.1	-	Spehar et al., 1999
Hydra, <i>Hydra sp.</i>	X	W,E	phenanthrene (85-01-8)	4.57	FT	M	96	0.539	0.539	11.2	11.2	15.5	Call et al., 1986
Annelid, <i>Lumbriculus variegatus</i>	X	I	phenanthrene (85-01-8)	4.57	FT	M	>419	>2.35	>2.35	>49.0	-	-	Call et al., 1986
Annelid, <i>Lumbriculus variegatus</i>	A	I	fluoranthene (206-44-0)	5.08	FT	M	>178	>0.880	>0.880	>56	>52.4	>52.4	Spehar et al., 1999
Snail, <i>Mudalia potosensis</i>	X	E	fluorene (86-73-7)	4.21	S	U	>1900 ^g (5600)	>11.4	>11.4	>108	>108	>108	Finger et al., 1985
Snail, <i>Aplexa hypnorum</i>	X	E	acenaphthene (83-32-9)	4.01	FT	M	>2040	>13.2	>13.2	>81.8	>81.8	>81.8	Holcömbe et al., 1983
Snail, <i>Physa heterostrophia</i>	X	E	fluoranthene (206-44-0)	5.08	S	U	137	0.677	0.677	43.2	43.2	43.2	Horne and Oblad, 1983
Snail, <i>Physella virgata</i>	A	E	fluoranthene (206-44-0)	5.08	FT	M	>178	>0.880	>0.880	>56	>56	>56	Spehar et al., 1999
Cladoceran, <i>Daphnia magna</i>	X	W	naphthalene (91-20-3)	3.36	S	U	8570	66.9	-	-	-	-	U.S. EPA, 1978
Cladoceran, <i>Daphnia magna</i>	J	W	naphthalene (91-20-3)	3.36	S	U	4723	36.9	-	-	-	-	Abernethy et al., 1986
Cladoceran, <i>Daphnia magna</i>	X	W	naphthalene (91-20-3)	3.36	S	M	2160	16.9	34.6	51.0	-	-	Millemann et al., 1984
Cladoceran, <i>Daphnia magna</i>	J	W	1-methyl naphthalene (90-12-0)	3.84	S	U	1420	9.99	9.99	42.2	-	-	Abernethy et al., 1986

Chemical	CAS ^A	Class ^B	K _{ow} ^C	MW ^D	MV ^E	S ^F
1-tridecanol*	112709	ao	5.75	200.36	224	0.0000793
decane*	124185	al	6.56	142.28	229	0.000000300

*Chemical is not included: LC50 > S.

^ACAS=Chemical abstract number

^BClass: ao=alcohol, ar=aromatic, ha=halogenated, et=ether, al=aliphatic, ke=ketone, pah=PAH

^CK_{ow}=log₁₀(K_{ow});

^DMW=molecular weight (gm/mol);

^EV=molar volume (cm³/mol);

^FS=aqueous solubility(mol/L)

Chemical	CAS ^A	Class ^B	K _{ow} ^C	MW ^D	MV ^E	S ^F
acenaphthene	83329	pah	4.01	154.21	140	0.000100
2,5-dimethyl-2,4-hexadiene	764136	al	4.10	110.20	146	0.000133
methyl cyclohexane	108872	al	4.10	98.19	128	0.000155
1,2,4,5-tetramethylbenzene	95932	ar	4.11	134.22	152	0.000159
hexane	110543	al	4.12	86.18	132	0.000131
1,3-diethylbenzene	141935	ar	4.17	134.22	156	0.000135
1-decanol	112301	ao	4.19	158.28	192	0.00181
p-tert-butyltoluene	98511	ar	4.26	148.25	173	0.0000995
diphenylether	101848	et	4.36	170.21	152	0.0000595
amylbenzene	538681	ar	4.52	148.25	173	0.0000502
phenanthrene	85018	pah	4.57	178.23	161	0.0000340
1,2,4,5-tetrachlorobenzene	95943	ar,ha	4.64	215.89	136	0.0000151
1,2,3,4-tetrachlorobenzene	634662	ar,ha	4.64	215.89	136	0.0000145
1,2,3,5-tetrachlorobenzene	634902	ar,ha	4.64	215.89	136	0.0000148
1-undecanol	112425	ao	4.70	172.31	207	0.000640
pyrene	129000	pah	4.92	202.26	182	0.0000120
9-methylanthracene	779022	pah	5.01	192.26	175	0.00000980
fluoranthene	206440	pah	5.08	202.26	197	0.0000102
1-dodecanol	112538	ao	5.20	186.34	223	0.000238
pentachlorobenzene	608935	ar,ha	5.32	250.34	147	0.00000218
octane*	111659	al	5.34	114.23	164	0.00000625

Chemical	CAS ^A	Class ^B	K _{ow} ^C	MW ^D	MV ^E	S ^F
2-dodecanone	6175491	ke	3.43	184.32	223	0.0357
cumene	98828	ar	3.49	120.19	140	0.000762
pentane	109660	al	3.50	72.15	116	0.000592
1,2-dibromobenzene	585539	ar,ha	3.56	235.92	119	0.000196
1,5-cyclooctadiene	111784	al	3.61	108.18	130	0.000386
1-nonanol	143088	ao	3.63	144.26	175	0.00552
1,2,4-trimethylbenzene	95636	ar	3.65	120.19	138	0.000487
n-propylbenzene	103651	ar	3.67	120.19	140	0.000467
dipentyl ether	693652	et	3.69	158.28	202	0.000757
1,3,5-trimethylbenzene	108678	ar	3.69	120.19	140	0.000414
hexachloroethane	67721	al,ha	3.73	236.74	132	0.0000936
2,4-dichlorotoluene	95738	ar,ha	3.79	161.03	129	0.000457
1-methylnaphthalene	90120	pah	3.84	142.20	140	0.000280
2-methylnaphthalene	91576	pah	3.86	142.20	141	0.000270
2-chloronaphthalene	91587	pah,ha	3.88	162.62	136	0.000100
1-chloronaphthalene	90131	pah,ha	3.88	162.62	136	0.000100
3,4-dichlorotoluene	95750	ar,ha	3.88	161.03	129	0.000120
biphenyl	92524	ar	3.91	154.21	150	0.000216
1,3,5-trichlorobenzene	108703	ar,ha	3.97	181.45	125	0.0000933
1,2,3-trichlorobenzene	87616	ar,ha	3.98	181.45	124	0.0000870
1,2,4-trichlorobenzene	120821	ar,ha	4.00	181.45	126	0.0000886

Chemical	CAS ^A	Class ^B	K _{ow} ^C	MW ^D	MV ^E	S ^F
1,3,5-cycloheptatriene	544252	al	2.77	92.14	104	0.00377
trichloroethylene	79016	al,ha	2.81	131.39	90.0	0.00360
di-n-butyl ether	142961	et	2.89	130.23	170	0.00614
t-1,2-dichlorocyclohexane	822866	al,ha	2.90	153.05	128	0.00162
pentachloroethane	76017	al,ha	2.95	202.29	121	0.00111
2,4-hexadiene	592461	al	2.98	82.145	115	0.00237
butylphenyl ether	1126790	et	3.00	150.22	160	0.000790
benzophenone	119619	ke	3.05	182.22	163	0.000480
ethylbenzene	100414	ar	3.06	106.17	123	0.00219
2,3-dimethyl-1,3-butadiene	513815	al	3.06	82.145	121	0.00162
2-undecanone	112129	ke	3.08	170.29	207	0.0459
1-octanol	118875	ao	3.10	130.23	158	0.0161
3-chlorotoluene	108418	ar,ha	3.12	126.59	118	0.000834
4-chlorotoluene	106434	ar,ha	3.13	126.59	118	0.000817
o-xylene	95476	ar	3.13	106.17	121	0.00191
m-xylene	108383	ar	3.19	106.17	124	0.00154
p-xylene	106423	ar	3.21	106.17	124	0.00146
1,4-dichlorobenzene	106467	ar,ha	3.24	147.00	113	0.000581
3,5,5-trimethyl-1-hexanol	3452979	ao	3.29	144.26	172	0.0117
1,2-dichlorobenzene	95501	ar,ha	3.31	147.00	113	0.000507
1,3-dichlorobenzene	541731	ar,ha	3.31	147.00	115	0.000524
napthalene	91203	pah	3.36	128.17	125	0.00110
cyclohexane	110827	al	3.38	84.16	109	0.000919
tetrachloroethylene	127184	al,ha	3.38	165.83	99.0	0.000710

Chemical	CAS ^A	Class ^B	K _{ow} ^C	MW ^D	MV ^E	S ^F
benzene	71432	ar	2.00	78.11	89.0	0.0260
1-hexanol	111273	ao	2.02	102.18	125	0.159
2-octanone	111137	ke	2.02	128.21	157	0.111
1-chloro-3-bromopropane	109706	al,ha	2.04	157.44	100	0.0184
5-methyl-3-heptanone	541855	ke	2.05	128.21	156	0.111
anisole	100663	ar	2.06	108.14	111	0.0148
2,6-dimethyl-2,5-heptadiene	504201	ke	2.07	138.21	164	0.0171
t-1,2-dichloroethylene	156605	al,ha	2.10	96.94	81.0	0.0202
1,2,3-trichloroethane	96184	al,ha	2.13	147.43	107	0.0177
1,1-dichloroethylene	75354	al,ha	2.19	96.94	81.0	0.0141
1,3-dibromopropane*	109648	al,ha	2.24	201.9	103	0.00930
bromoform	75252	al,ha	2.25	252.73	88.0	0.00650
1,1,2,2-tetrachloroethane	79345	al,ha	2.31	167.85	106	0.0181
1,4-dichlorobutane	110565	al,ha	2.33	127.01	113	0.00990
1,1-dichloropropane	78999	al,ha	2.36	112.99	101	0.00790
2-nonanone	821556	ke	2.38	142.24	174	0.0801
1,1,1-trichloroethane	71556	al,ha	2.38	133.4	101	0.00662
1,1,1,2-tetrachloroethane	630206	al,ha	2.43	167.85	110	0.0050
5-nonanone	502567	ke	2.44	142.24	174	0.0740
1-heptanol	111706	ao	2.57	116.2	142	0.0487
chlorobenzene	108907	ar,ha	2.58	112.56	102	0.00320
2-ethyl-1-hexanol	104767	ao	2.58	130.23	155	0.132
bicyclo(2,2,1)hepta-2,5-diene	121460	al	2.60	92.14	102	0.00490
toluene	108883	ar	2.62	92.14	107	0.00600
styrene	100425	ar	2.72	104.15	116	0.00550
tetrachloromethane	56235	al,ha	2.73	153.82	97.0	0.00248
2-decanone	693549	ke	2.73	156.27	190	0.0599
bromobenzene	108861	ar,ha	2.75	157.01	106	0.00196
cyclopentane	278923	al	2.76	70.134	95.0	0.00260
1,5-dichloropentane	628762	al,ha	2.76	141.04	130	0.00286

Chemical	CAS ^A	Class ^B	K _{ow} ^C	MW ^D	MV ^E	S ^F
2-methyl-2-butanol	75854	ao	1.03	88.15	110	1.62
2-n-butoxyethanol	111762	ao	1.05	118.17	131	8.78
diethyleneglycolmono-n-butylether	112345	et	1.09	162.23	170	40.0
3,3-dimethyl-2-butanone	75978	k	1.09	100.16	125	0.954
diethyl ether	60297	et	1.15	74.122	105	1.16
4-methoxy-4-methyl-2-pentane	107700	k	1.17	130.19	143	41.5
4-methyl-2-pentanone	108101	k	1.17	100.16	124	0.862
dichloromethane	75092	al,ha	1.18	84.93	65.0	0.211
t-butylmethyl ether	1634044	et	1.20	88.149	122	9.04
cyclohexanol	108930	ao	1.29	100.16	103	1.61
2-hexanone	591786	k	1.29	100.16	124	0.598
1,2-dichloroethane	107062	al,ha	1.40	98.96	79.0	0.114
1-pentanol	71410	ao	1.49	88.15	109	0.581
3-methyl-3-pentanol	77747	ao	1.49	102.18	125	3.79
2-phenoxyethanol	122996	ao	1.50	138.17	122	0.173
2,2,2-trichloroethanol	115208	ao	1.61	149.4	93.0	48.4
4-methyl-2-pentanol	108112	ao	1.66	102.18	126	2.25
3-hexanol	623370	ao	1.66	102.18	125	2.18
2-heptanone	110430	ke	1.67	114.19	141	0.312
5-methyl-2-hexanone	110123	ke	1.68	114.19	141	0.271
2,4-dimethyl-3-pentanol	600362	ao	1.78	116.2	140	3.05
6-methyl-5-heptene-2-one	110930	ke	1.82	126.2	151	0.487
2-hexanol	626937	ao	1.83	102.18	126	1.13
1,3-dichloropropane	142289	al,ha	1.84	112.99	97.0	0.0363
1,2-dichloropropane	78875	al,ha	1.86	112.99	99.0	0.0342
diisopropyl ether	108203	et	1.87	102.18	138	0.0918
chloroform	67663	al,ha	1.91	119.38	81.0	0.0319
1,1,2-trichloroethane	79005	al,ha	1.91	133.4	94.0	0.0369
1,4-dimethoxybenzene	150787	ar	1.95	138.165	132	0.0250
2,6-dimethoxytolunene	5673074	ar	1.99	152.19	147	0.0283

Appendix B. Chemicals which comprise the acute toxicity database for narcosis chemicals in Section 2 of this document. Table from Di Toro et al. (2000).

Chemical	CAS ^A	Class ^B	K_{ow} ^C	MW ^D	MV ^E	S ^F
triethylene glycol	112276	ao	-1.48	150.17	131	-
methanol	67561	ao	-0.715	32.04	41.0	13.5
2,4-pentanedione*	123546	k	-0.509	100.12	100	7.87
ethanol	64175	ao	-0.234	46.07	59.0	11.9
acetone	67641	k	-0.157	58.08	74.0	13.71
2-chloroethanol*	107073	ao	-0.048	80.51	65.0	9.09
2-(2-ethoxyethoxy)ethanol	111900	ao	0.011	134.17	111	-
1-chloro-2-propanol*	127004	ao	0.156	94.54	84.0	44.8
1,3-dichloro-2-propanol*	96231	ao	0.165	128.99	91.0	6.30
2-methyl-2,4-pentanediol	107415	ao	0.246	118.17	120	43.0
2-butanone	78933	k	0.316	72.11	90.0	2.81
2-propanol	67630	ao	0.341	60.10	77.0	13.6
3-chloro-1-propanol*	627305	ao	0.363	94.54	82.0	2.00
1-propanol	71238	ao	0.399	60.10	75.0	11.2
cyclopentanone	120923	k	0.453	84.12	89.0	1.11
2-methyl-2-propanol	75650	ao	0.663	74.12	95.0	16.5
methyl chloride	74873	al,ha	0.677	50.49	56.0	0.0666
2-butanol	78922	ao	0.717	74.12	93.0	14.9
methyl bromide*	74839	al,ha	0.791	94.94	57.0	0.154
3-methyl-2-butanone	563804	k	0.792	86.13	108	1.32
2,3-dibromopropanol*	96139	ao	0.819	217.90	96.0	5.97
cyclohexanone	108941	k	0.827	98.14	103	0.445
cyclopentanol	96413	ao	0.849	86.13	89.0	5.19
2-methyl-1-propanol	78831	ao	0.858	74.12	93.0	10.6
4-methyl-3-pente-2-one	141797	k	0.867	98.14	118	2.68
2-pentanone	107879	k	0.877	86.13	107	1.03
1-butanol	71363	ao	0.946	74.12	92.0	3.03
3-pentanone	96220	k	0.954	86.13	108	0.849

1 $\Sigma\text{ESGTU}_{\text{FCV,TOT}}$ for each sediment (plotted as circles in Figure 6-2) was determined by multiplying the
2 sediment-specific $\Sigma\text{ESGTU}_{\text{FCV,13}}$ values by 11.5 and by multiplying the sediment-specific $\Sigma\text{ESGTU}_{\text{FCV,23}}$
3 by 4.14 (Table 6-1). The 95% limits on the $\Sigma\text{ESGTU}_{\text{FCV,TOT}}$ estimated from the $\Sigma\text{ESGTU}_{\text{FCV,13}}$
4 exceeded 1.0 for 35.5% of the 1992 sediments and the 95% limits on the $\Sigma\text{ESGTU}_{\text{FCV,TOT}}$ estimated
5 from the $\Sigma\text{ESGTU}_{\text{FCV,23}}$ exceeded 1.0 for 23.7% of the 2001 sediments. Therefore, if the 95%
6 uncertainty ratios are applied to the $\Sigma\text{ESGTU}_{\text{FCV,13}}$ or the $\Sigma\text{ESGTU}_{\text{FCV,23}}$ the predicted $\Sigma\text{ESGTU}_{\text{FCV,TOT}}$
7 for about one-third of the sediments are in excess of the ESG for PAH mixtures of 1.0 $\Sigma\text{ESGTU}_{\text{FCV}}$.
8 This strongly suggests that new monitoring programs should quantify a minimum of the 34 PAHs
9 monitored by the U.S. EPA EMAP program. It is important to repeat that at present the uncertainty of
10 using the 34 PAHs to estimate the total toxicological contributions of the unmeasured PAHs is unknown
11 and needs additional research.

12 13 6.3 INTERPRETING ESGs IN COMBINATION WITH TOXICITY TESTS

14
15 Sediment toxicity tests provide an important complement to ESGs in interpreting overall risk
16 from contaminated sediments. Toxicity tests have different strengths and weaknesses compared to
17 chemical-specific guidelines, and the most powerful inferences can be drawn when both are used
18 together.

19 Unlike chemical-specific guidelines, toxicity tests are capable of detecting any toxic chemical,
20 if it is present in toxic amounts; one does not need to know what the chemicals of concern are to
21 monitor the sediment. Toxicity tests are also useful for detecting the combined effect of chemical
22 mixtures, if those effects are not considered in the formulation of the applicable chemical-specific
23 guideline.

24 On the other hand, toxicity tests have weaknesses also; they provide information only for the

1 species tested, and also only for the endpoints measured. This is particularly critical given that most
2 sediment toxicity tests conducted at the time of this writing measure primarily short-term lethality;
3 chronic test procedures have been developed and published for some species, but these procedures are
4 more resource-intensive and have not yet seen widespread use. In contrast, chemical-specific
5 guidelines are intended to protect most species against both acute and chronic effects.

6 Many assessments may involve comparison of sediment chemistry (e.g., using ESG values) and
7 toxicity test results. In cases where results using these two methods agree (either both positive or both
8 negative), the interpretation is clear. In cases where the two disagree, the interpretation is more
9 complex; some investigators may go so far as to conclude that one or the other is "wrong," which is
10 not necessarily the case.

11 Individual ESGs consider only the effects of the chemical or group of chemicals for which they
12 are derived. For this reason, if a sediment shows toxicity but does not exceed the ESG for a chemical
13 of interest, it is likely that the cause of toxicity is a different chemical or chemicals.

14 In other instances, it may be that an ESG is exceeded but the sediment is not toxic. As
15 explained above, these findings are not mutually exclusive, because the inherent sensitivity of the two
16 measures is different. ESGs are intended to protect relatively sensitive species against both acute and
17 chronic effects, whereas toxicity tests are run with specific species that may or may not be sensitive to
18 chemicals of concern, and often do not encompass the most sensitive endpoints (e.g., chronic survival,
19 growth or reproduction). It is also possible for a sediment above the ESG to be non-toxic if there are
20 site-specific conditions that run counter to the equilibrium partitioning model and its assumptions (see
21 Section 7.2).

22 The first step in interpreting this situation is to consider the magnitude of the ESG exceedance
23 and the sensitivity of the test organism and endpoint to the suspect chemical. For example, the acute-
24 chronic ratio used for the PAH ESG is 4.16 (Section 3.3.7); as such, if $\Sigma \text{ESG}_{\text{TCV}} = 4$, one would

1 expect lethal effects only for highly sensitive species. Between $\Sigma\text{ESGTU}_{\text{FCV}}$ of 1 and 4, one would
2 expect only chronic effects, unless the test species was unusually sensitive. If $\Sigma\text{ESGTU}_{\text{FCV}}$ for PAHs
3 was 2, for example, one would not generally expect to see lethality from PAHs in short term sediment
4 lethality tests.

5 A more precise method for evaluating the results of toxicity tests is to calculate effect
6 concentrations in sediment that are species specific. For species contained in the toxicity data for the
7 PAH ESG (Section 3.2.1), effect concentrations in sediment can be calculated that are specific for that
8 organism (using procedures in Section 4). These values could then be used to directly judge whether
9 the absence of toxicity in the toxicity test would be expected from the corresponding level of sediment
10 contamination.

11 If the exceedance of the PAH ESG is sufficient that one would expect effects in a toxicity test
12 but they were not observed, it is prudent to evaluate the partitioning behavior of the chemical in the
13 sediment. This is done by isolation of interstitial water from the sediment and analyzing it for the same
14 PAHs measured in the solid phase. Predicted concentrations of chemicals in the interstitial water can
15 be calculated from the measured concentrations in the solid phase (normalized to organic carbon)

$$16 \quad C_d = C_{\text{OC}} / K_{\text{OC}} \quad (6-4)$$

17
18
19 For chemicals with $\log_{10}K_{\text{OW}}$ greater than 5.5, corrections for DOC binding in the interstitial
20 water will be necessary

$$21 \quad C_{\text{d, IW}} = C_{\text{IW, OC}} / K_{\text{DOC}} \quad (6-5)$$

22
23
24 If the measured chemical in the interstitial water is substantially less (e.g., 2-3 fold lower or

more), it suggests that the organic carbon in that sediment may not partition similarly to more typical organic carbon, and derivation of site-specific ESGs based on interstitial water may be warranted (U.S.EPA, 2000f).

6.4 PHOTO-ACTIVATION

6.4.1 Overview

Research over the last decade has shown that the presence of ultraviolet (UV) light can greatly enhance the toxicity of many PAHs. This "photo-activated" toxicity has been shown to cause rapid, acute toxicity to several freshwater and marine species including fish, amphibians, invertebrates, plants and phytoplankton (Bowling et al., 1983; Cody et al., 1984; Kagan et al., 1984; Landrum et al., 1984a,b; Oris et al., 1984; Allred and Giesy, 1985; Kagan et al., 1985; Oris and Giesy, 1985, 1986, 1987; Gala and Giesy, 1992; Huang et al., 1993; Gala and Giesy, 1994; Ren et al., 1994; Arfsten et al., 1996; Boese et al., 1997; Huang et al., 1997; McConkey et al., 1997; Pelletier et al., 1997; Hatch and Burton, 1998; Spehar et al., 2000). Depending on the organism and exposure regime, photo-activation can increase toxicity of PAH by one to four orders of magnitude over that caused by narcosis.

The mechanism for phototoxicity has been related to the absorption of ultraviolet radiation (UV) by the conjugated bonds of selected PAH molecules



This excites the PAH molecules to a triplet state (PAH*) which rapidly transfers the absorbed

1 energy to ground state molecular oxygen (O_2) forming excited singlet oxygen intermediaries (O_2^*)
2 (Newsted and Giesy, 1987). Although extremely short-lived (2 to 700 μs), oxygen free radicals are
3 highly oxidizing and can cause severe tissue damage upon contact. Despite the many different parent
4 PAHs and related alkylated forms, not all PAHs induce photo-activated toxicity. Those PAHs that are
5 photo-activated can be predicted using various molecular physical-chemical variables (Newsted and
6 Giesy, 1987; Oris and Giesy, 1987); however, the Highest Occupied Molecular Orbital - Lowest
7 Unoccupied Molecular Orbital gap model (HOMO-LUMO) has been the most successful (Mekenyan et
8 al. 1994a,b; Veith et al. 1995a,b; Ankley et al. 1996; Ankley et al. 1997). As research on the nature
9 of photo-activated toxicity has evolved, certain key elements of this phenomena have been better
10 defined including interactions of UV and PAH dose, effects of temperature, humic substances,
11 organism behavior, turbidity, dissolved oxygen, and mixtures (Oris et al., 1990; McCloskey and Oris,
12 1991; Ankley et al., 1995, 1997; Ireland et al., 1996; Hatch and Burton, 1998).

13 Eight studies have been performed with sediments contaminated with PAHs to assess the
14 importance of photo-activated toxicity in the benthos (Davenport and Spacie, 1991; Ankley et al.,
15 1994; Monson et al., 1995; Sibley et al., 1997; Swartz et al., 1997; Boese et al., 1998, 1999; Kosian et
16 al., 1998; Spehar et al., 2000). These studies conclude that photo-activated toxicity may occur in
17 shallow water environments; however, the magnitude of these effects are not as well characterized as in
18 water-only exposures and are probably not as dramatic as those observed in the water column.
19 Comparisons by Swartz et al. (1995) suggest that responses of benthic communities in PAH-
20 contaminated sites correlate well with the toxicity that is predicted based on narcosis, suggesting that
21 photo-activation was not a major confounding factor for those environments. However, Boese et al.
22 (1997) and Pelletier et al. (2000a) show that life history of benthic organisms is critical to assessing
23 whether or not photo-activated toxicity will occur. For example, several marine species that frequently
24 encounter ultraviolet radiation during low tide are not vulnerable to photo-activated toxicity due to light

1 protective adaptation (e.g., shells, pigments, borrowing). Additionally, there is evidence that maternal
2 transfer of PAHs from benthic adult bivalves to pelagic embryos does occur (Pelletier et al., 2000b).

3 4 6.4.2 Implications to Derivation of ESG

5
6 Because the total PAH ESG derived here is based on narcosis, additional toxicity caused by
7 photo-activation would cause the ESG to be underprotective. At present, the magnitude of potential
8 errors can not be specifically quantified, but are probably significant primarily for habitats in very
9 shallow or very clear water. This is because of the rapid attenuation of ultraviolet radiation in the
10 water column (Pickard and Emery 1982; Wetzel, 1983). For example, <25% of incident UV
11 penetrates below the first meter of water in productive aquatic systems. In areas where PAH-
12 contaminated sediments are present in shallow environments the risk of photo-activated toxicity is
13 greater and a site-specific ESG may need to be generated that considers this potential risk.

14 15 6.5 TERATOGENICITY AND CARCINOGENICITY

16
17 This subsection presents an analysis intended to determine if the ESG for PAH mixtures of 1.0
18 $\Sigma\text{ESGTU}_{\text{FCV}}$ is protective for non-narcosis modes of toxic action of individual PAHs. Published
19 articles were screened for applicable data on teratogenic (Appendix E) and carcinogenic (Appendix F)
20 effects of individual PAHs and their mixtures. Five laboratory studies with benzo(a)pyrene (BaP),
21 predominantly water exposures, and one with anthracene were selected for analysis of teratogenic
22 effects; two laboratory studies with BaP were selected for analysis of carcinogenic effects (Table 6-3).
23 In the teratogen studies, typically radio-labeled BaP was used to quantify the accumulation of the PAH
24 and its metabolites in fish ranging in age from embryo to adults. The water PAH concentrations

1 associated with teratogenic and carcinogenic effects were generally high and steady-state was not
2 always achieved. Hence, the solubility limit in water for BaP of 3.81 $\mu\text{g/L}$ was exceeded in 6 of 8
3 experiments (Table 6-3). In contrast, for seven of the experiments, the BaP concentration in eggs or
4 fish tissue was the observed effect concentration. The theoretical solubility-limited maximum of 3840
5 $\mu\text{g BaP/g lipid}$ was exceeded only in one of the experiments. For these reasons, when the
6 concentration of BaP plus metabolites was measured in the eggs or tissue of the organism, this
7 concentration was considered the most valid representation of the true observed exposure concentration
8 and the water concentration was not used in further analysis. Elutriates from crude oil contained non-
9 PAH compounds and the relationship of total PAH concentrations in the study vs total PAH as defined
10 in this document were difficult to determine in the Carls et al. (1999) study; therefore, these data were
11 also excluded from this analysis.

12 As indicated in Table 6-3 and Appendix F, the database for carcinogenic effects of PAHs on
13 aquatic (fish) species from laboratory studies is limited. Most of the available data are from studies of
14 epizootic outbreaks of neoplasia (tumors) from highly contaminated field sites such as the Black River,
15 Ohio (see Baumann, 1998 for review) or Puget Sound, WA (Malins et al., 1987, Myers et al., 1990),
16 to mention only a notable few. The applicability of these field studies to a causal relationship between
17 carcinogenic effects observed and PAH concentrations is limited by the possible interactive effects of
18 the PAHs with PCBs and other simultaneously occurring chemicals. The bulk of laboratory
19 experimental evidence for carcinogenic effects of PAHs is based on the distribution of neoplasms in
20 fish species exposed to PAH-enriched sediment extracts (Black, 1983; Metcalfe et al., 1988; Fabacher
21 et al., 1991), dietary exposures or inter-peritoneal injection (Hendricks et al., 1985), or intermittent
22 water exposures of 7,12-dimethylbenzanthracene (Schultz and Schultz, 1982). These studies are listed
23 in Appendix F for completeness, but were not included in Table 6-3 for further analysis. This is
24 because the exposure regime or concentrations of individual or mixtures of PAHs were not provided in

1 sufficient detail to permit critical measured sediment concentrations, or sediment concentrations derived
2 from concentrations in water or tissue, to be compared to the observed carcinogenic effects. The study
3 with 7,12-dimethylbenzanthracene (Schultz and Schultz, 1982) was not considered for analysis because
4 this PAH is not commonly measured as part of the environmental monitoring programs (see Table 6-2).

5 A far more extensive database exists on the influence of PAHs on various aspects of tumor
6 biology, such as PAH-DNA adduct formation and phase I (oxidation, reduction, and hydrolysis
7 reactions) and phase II (glucuronidation and glutathione conjugation) metabolism of individual
8 compounds. However, as indicative of cytotoxicity as these biomarkers may or may not be, they have
9 been excluded from the analysis for the explicit purposes of this subsection. The methods of PAH
10 exposure that were useful for this analysis were aqueous (Hannah et al., 1982; Hose et al., 1982, 1984;
11 Winkler et al., 1983; Goddard et al., 1987; Hawkins et al., 1988, 1990), maternal (Hall and Oris,
12 1991), or inter-peritoneal injection of adult English sole (*Parophrys vetulus*) followed by measurement
13 of concentrations in embryos (Hose et al., 1981).

14 15 6.5.1 Calculations

16
17 When the measured concentration of the PAH dissolved in water (C_d ; $\mu\text{g/L}$) associated with a
18 teratogenic or carcinogenic effect was available it was multiplied by its K_{oc} (L/kg_{oc}) $\times 10^{-3}$ to derive an
19 equivalent effect concentration in sediment (C_d -derived C_{oc} ; $\mu\text{g/g}_{oc}$), as per the EqP methodology
20 (Table 6-3; Appendix E and F). When the measured concentration of the PAH in eggs or tissue (C_L ;
21 $\mu\text{g PAH/g lipid}$) associated with an effect was available, its equivalent effect concentration in sediment
22 (C_L -derived C_{oc} ; $\mu\text{g/g}_{oc}$) was calculated using the following equation from Di Toro and McGrath
23 (2000)

$$\log_{10}C_{OC} = 0.00028 + \log_{10}C_L + 0.038 \log_{10}K_{OW} \quad (6-7)$$

6.5.2 Critical Sediment Concentrations for Teratogenic and Carcinogenic Effects versus ESGs for PAH Mixtures

The critical sediment concentrations (i.e., C_d or C_L -derived C_{OC}) that would be expected to cause teratogenic or carcinogenic effects on the five freshwater and three saltwater fishes exposed to BaP ranged from 57 to 8,937 $\mu\text{g/g}_{OC}$; the only C_{OC} for anthracene was 219 $\mu\text{g/g}_{OC}$ (Table 6-3). The majority of C_{OC} values were derived using concentrations measured in fish eggs. Six of the nine C_{OC} concentrations for BaP were less than the solubility-limited maximum concentration of 3,840 $\mu\text{g/g}_{OC}$. The C_{OC} value of 8,937 $\mu\text{g/g}_{OC}$ is retained because the concentrations in the eggs probably included metabolites of BaP that are quantified as total BaP equivalents in the radio-label analysis. The C_{OC} values for individual PAHs in sediments were then compared to total PAH concentrations in monitored field sediments to determine if teratogenic or carcinogenic effects might occur in sediments having $<1.0 \Sigma\text{ESGTU}_{FCV}$. This analysis was used to determine if the ESG derived from the narcosis mode of action was protective of teratogenic or carcinogenic effects.

The combined databases from the U.S. EPA EMAP (U. S. EPA 1996b, 1998) and Elliott Bay (Ozretich et al., 2000b) sediment monitoring programs were used to compare the BaP (Figure 6-3A) or anthracene (Figure 6-4A) concentration of 539 sediment samples where 34 PAHs, or 33 PAHs for Elliott Bay, were measured versus the ΣESGTU_{FCV} for all PAHs measured in those sediments. The lowest critical sediment concentration for teratogenic or carcinogenic effects is indicated with a solid line at 57 $\mu\text{g/g}_{OC}$ for BaP and at 219 $\mu\text{g/g}_{OC}$ for anthracene. None of the sediments having $<1.0 \Sigma\text{ESGTU}_{FCV}$ contained BaP or anthracene at concentrations likely to cause the teratogenic or carcinogenic effects reported in Table 6-3. The same database of PAH concentrations in field

sediments was used to calculate the sediment-specific BaP: Σ ESGTU_{FCV} ratio and the sediment-specific anthracene: Σ ESGTU_{FCV} ratio. The total PAH concentration in each of the 539 sediments was multiplied by its sediment-specific ratio to determine the BaP or anthracene concentration for the sediment if the Σ ESGTU_{FCV} was equal to 1.0. Probability plots of the calculated concentrations for the BaP and anthracene at 1.0 Σ ESGTU_{FCV} are in Figures 6-3B and 6-4B, respectively. The solid lines represent the critical sediment concentration for each respective PAH. None of the sediments for anthracene and 3.53% of the sediments for BaP would be expected to produce teratogenic or carcinogenic effects if the ESG for PAH mixtures in these sediments were equal to 1.0 Σ ESGTU_{FCV}. The approach of examining these relationships individually with BaP or anthracene may be flawed because it may under-represent the teratogenic or carcinogenic contributions of other PAHs with the same mode of action in the PAH mixture. However, at present insufficient data are available to appropriately sum the contributions of multiple teratogenic or carcinogenic PAHs.

6.6 EQUILIBRIUM AND ESGs

Care must be used in application of ESGs in disequilibrium conditions. In some instances site-specific ESGs may be required to address this condition (U.S. EPA, 2000f). Guidelines based on EqP theory assume that nonionic organic chemicals are in equilibrium with the sediment and interstitial water, and that they are associated with the sediment primarily through adsorption into sediment organic carbon. In order for these assumptions to be valid, the chemical must be dissolved in interstitial water and partitioned into sediment organic carbon. The chemical must, therefore, be associated with the sediment for a sufficient length of time for equilibrium to be reached. With PAHs, the absence of toxicity when the ESG is exceeded may be because of the presence of less available PAHs associated with soot or coal particles in sediments (see discussion in Section 6.7). Alternatively,

$$\log_{10}C_{OC} = 0.00028 + \log_{10}C_L + 0.038 \log_{10}K_{OW} \quad (6-7)$$

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23 the absence of toxicity when the ESG is exceeded may be because of the presence of less available
24 PAHs associated with soot or coal particles in sediments (see discussion in Section 6.7). Alternatively,

1 disequilibrium exists, and ESG may be over-protective, when PAHs occur in sediments as undissolved
2 liquids or solids; although the use of solubility limited acceptable sediment concentrations should
3 adequately account for this.

4 In very dynamic locations, with highly erosional or depositional bedded sediments, the
5 partitioning of nonionic organic chemicals between sediment organic carbon and interstitial water may
6 only attain a state of near equilibrium. Likewise, nonionic organic chemicals with high $\log_{10}K_{ow}$ values
7 may come to equilibrium in clean sediment only after a period of weeks or months. Equilibrium times
8 are shorter for chemicals with low $\log_{10}K_{ow}$ values and for mixtures of two sediments with similar
9 organic carbon-normalized concentrations, each previously at equilibrium. This is particularly relevant
10 in tidal situations where large volumes of sediments are continually eroded and deposited, yet near
11 equilibrium conditions between sediment and interstitial water may predominate over large spatial
12 areas. For locations where times are sufficient for equilibrium to occur, near equilibrium is likely the
13 rule and disequilibrium uncommon. In many environments disequilibrium may occur intermittently,
14 but in those cases ESGs could be expected to apply when the disturbance abates, which can generally
15 be expected. In instances where long-term disequilibrium is suspected, application of site-specific
16 methodologies may be desirable (U.S. EPA, 2000f).

18 6.7 OTHER PARTITIONING PHASES

20 6.7.1 Overview

22 In general, laboratory studies with PAHs have shown the same partitioning behavior
23 demonstrated by many classes of nonpolar organic contaminants (Karickhoff et al., 1979; Means et al.,
24 1980; Di Toro et al., 1991). However, there are some data indicating that PAHs do not always follow

1 equilibrium partitioning behavior in the environment. Specifically, some studies have reported larger
2 partitioning coefficients for PAHs in field-collected sediments than is predicted based on laboratory or
3 SPARC-generated $\log_{10}K_{ow}/K_{oc}$ values (Prah1 and Carpenter, 1983; Socha and Carpenter, 1987;
4 Broman et al., 1990; McGroddy and Farrington, 1995; Maruya et al., 1996; McGroddy et al., 1996).
5 The observed differences in partitioning of PAHs may relate to differences in PAH sources with the
6 speculation that PAHs from combustion sources (e.g., soot or related materials, such as coal) may be
7 more strongly associated with the particulate phase than PAHs from some petrogenic sources (Readman
8 et al., 1984; Socha and Carpenter, 1987; McGroddy and Farrington, 1995; Chapman et al., 1996;
9 Maruya et al., 1996; McGroddy et al., 1996; Naes and Oug, 1997; Naes et al., 1998). The result is
10 that PAH concentrations in interstitial water are lower than laboratory or SPARC-generated K_{oc} values
11 and, presumably, exhibit correspondingly lower bioavailability. Several studies have proposed that the
12 lack of observable biological effects from sediments (and other samples) containing high concentrations
13 of presumably bioavailable PAHs is related to this phenomena (Farrington et al., 1983; Bender et al.,
14 1987; Knutzen, 1995; Chapman et al., 1996; Paine et al., 1996; Maruya et al., 1997).

15 The mechanisms causing these field observations of unusual PAH partitioning are not well
16 understood. One explanation proposes that PAHs condense into the soot matrix during particle
17 formation, and are thereby sterically inhibited from partitioning to interstitial water as would be
18 expected under equilibrium conditions. A second perspective assumes that the soot fraction represents
19 a second partitioning phase in addition to normal organic carbon. The partitioning of PAHs from this
20 phase approximate the equilibrium behavior assumed for normal organic carbon, but have a much
21 higher partitioning coefficient (K_{sc}) than biologically-derived organic carbon (represented by K_{oc})
22 (Gustafsson and Gschwend, 1997). Recently, a method was published for quantifying the combustion
23 or 'soot' phase in sediments (Gustafsson et al., 1997) for derivation of a fraction soot carbon (f_{sc}). The
24 soot phase can then be incorporated into an expanded partitioning equation with two partitioning terms

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23 or 'soot' phase in sediments (Gustafsson et al., 1997) for derivation of a fraction soot carbon (f_{sc}). The
24 soot phase can then be incorporated into an expanded partitioning equation with two partitioning terms

$$K_d = f_{OC}K_{OC} + f_{SC}K_{SC} \quad (6-8)$$

where, K_d is the partition coefficient for the expanded partitioning equation, f_{OC} and f_{SC} are the fraction organic carbon and fraction soot carbon, respectively, and K_{OC} and K_{SC} are the organic carbon and soot carbon partition coefficients.

6.7.2 Implications to Derivation of ESG

Irrespective of the mechanism, this issue has the potential to affect the predictive power and accuracy of the total PAH ESG. Since the presence of soot or related materials are associated with reduced concentrations of PAH in interstitial water, one would presume that this results in decreased bioavailability of PAHs, a phenomenon demonstrated by West et al. (2000). This, in turn, would make the total PAH ESG derived here overprotective, because the K_{OC} -based partitioning model would overpredict chemical activity and, therefore, concentrations of PAH in interstitial water and organisms.

Nonetheless, empirical data suggest that this error may not be pervasive; most applications of the PAH mixture narcosis model to toxicity data for field-collected sediments show good predictive ability for the ESG (see Section 5.3). This may be because most sediments that are sufficiently contaminated to cause narcosis are contaminated by PAH sources that exhibit normal partitioning behavior, such as creosote and other petrogenic sources. In their study of PAH-contaminated sediments, Ozretich et al. (2000b) found that discrepancies between measured and predicted partitioning behavior predominated in sediments with lower PAH concentrations, while those with higher PAH concentrations showed partitioning behavior closer to that predicted from published K_{OW}/K_{OC} relationships. This differential behavior was attributed to the presence of two PAH sources, with creosote being the source causing the highest levels of contamination and toxicity.

In cases where it is suspected that soot, coal, or other materials may be causing unusual partitioning, direct measurement of PAH concentrations in interstitial water may be used to evaluate this possibility and, where necessary, derive site-specific sediment guidelines which account for local differences in partitioning behavior.

6.8 AQUEOUS SOLUBILITY UNDER NON-STANDARD CONDITIONS

It has been long established that organic compounds are generally less soluble in aqueous solutions at colder temperatures than at warmer, and in salt solutions such as seawater, than in freshwater, a phenomenon termed the salting-out effect (May, 1980; Schwarzenbach et al., 1993; Xie et al., 1997). Setschenow (1889) derived an empirical relationship for the magnitude of the salting-out effect:

$$\log_{10}(S_0 / S_{\%o}) = K_S C_{\text{salt}} \quad (6-9)$$

where S_0 and $S_{\%o}$ are the aqueous solubilities of the solute in fresh and saltwater (in mol/L at temperature ($^{\circ}\text{C}$), respectively, K_S is the Setschenow constant (L/mol) for the salt solution and the solute of interest, and C_{salt} is the molar salt concentration. A one molar salt solution (NaCl) is approximately equivalent to 48‰ sea water (Owen and Brinkley, 1941), and K_S was found to be essentially invariant with temperatures from 1 to 30°C , averaging 0.28 ± 0.02 (mean \pm SE) (May, 1980) for 9 PAHs. Temperature has been shown to have a non-linear effect on PAHs solubilities (May, 1980). Concentrations of 9 compounds: naphthalene, fluorene, phenanthrene, 1-methylphenanthrene, anthracene, fluoranthene, pyrene, benz(a)anthracene, and chrysene were computed for distilled water at temperatures between 5 and 30°C using the relationships of May (1980)

1
$$K_d = f_{oc}K_{oc} + f_{sc}K_{sc}$$
 (6-8)

2
3 where, K_d is the partition coefficient for the expanded partitioning equation, f_{oc} and f_{sc} are the fraction
4 organic carbon and fraction soot carbon, respectively, and K_{oc} and K_{sc} are the organic carbon and soot
5 carbon partition coefficients.

6
7 6.7.2 Implications to Derivation of ESG

8
9 Irrespective of the mechanism, this issue has the potential to affect the predictive power and
10 accuracy of the total PAH ESG. Since the presence of soot or related materials are associated with
11 reduced concentrations of PAH in interstitial water, one would presume that this results in decreased
12 bioavailability of PAHs, a phenomenon demonstrated by West et al. (2000). This, in turn, would make
13 the total PAH ESG derived here overprotective, because the K_{oc} -based partitioning model would
14 overpredict chemical activity and, therefore, concentrations of PAH in interstitial water and organisms.

15 Nonetheless, empirical data suggest that this error may not be pervasive; most applications of
16 the PAH mixture narcosis model to toxicity data for field-collected sediments show good predictive
17 ability for the ESG (see Section 5.3). This may be because most sediments that are sufficiently
18 contaminated to cause narcosis are contaminated by PAH sources that exhibit normal partitioning
19 behavior, such as creosote and other petrogenic sources. In their study of PAH-contaminated
20 sediments, Ozretich et al. (2000b) found that discrepancies between measured and predicted
21 partitioning behavior predominated in sediments with lower PAH concentrations, while those with
22 higher PAH concentrations showed partitioning behavior closer to that predicted from published
23 K_{ow}/K_{oc} relationships. This differential behavior was attributed to the presence of two PAH sources,
24 with creosote being the source causing the highest levels of contamination and toxicity.

In cases where it is suspected that soot, coal, or other materials may be causing unusual partitioning, direct measurement of PAH concentrations in interstitial water may be used to evaluate this possibility and, where necessary, derive site-specific sediment guidelines which account for local differences in partitioning behavior.

6.8 AQUEOUS SOLUBILITY UNDER NON-STANDARD CONDITIONS

It has been long established that organic compounds are generally less soluble in aqueous solutions at colder temperatures than at warmer, and in salt solutions such as seawater, than in freshwater, a phenomenon termed the salting-out effect (May, 1980; Schwarzenbach et al., 1993; Xie et al., 1997). Setschenow (1889) derived an empirical relationship for the magnitude of the salting-out effect:

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where S_0 and $S_{\%}$ are the aqueous solubilities of the solute in fresh and saltwater (in mol/L at temperature ($^{\circ}\text{C}$), respectively, K_s is the Setschenow constant (L/mol) for the salt solution and the solute of interest, and C_{salt} is the molar salt concentration. A one molar salt solution (NaCl) is approximately equivalent to 48‰ sea water (Owen and Brinkley, 1941), and K_s was found to be essentially invariant with temperatures from 1 to 30°C , averaging 0.28 ± 0.02 (mean \pm SE) (May, 1980) for 9 PAHs. Temperature has been shown to have a non-linear effect on PAHs solubilities (May, 1980). Concentrations of 9 compounds: naphthalene, fluorene, phenanthrene, 1-methylphenanthrene, anthracene, fluoranthene, pyrene, benz(a)anthracene, and chrysene were computed for distilled water at temperatures between 5 and 30°C using the relationships of May (1980)

1 and are compared with the compounds' concentrations at 25°C (Figure 6-5). The least-squares
2 exponential representation of the data is as follows

$$3 \quad (S_0 / {}^{25}S_0) = 0.261 \times e^{0.0536t}, r^2 = 0.959 \quad (6-10)$$

5
6 where ${}^{25}S_0$ is the commonly reported solubility of a compound. Although naphthalene's solubility has
7 the least response to temperature of PAHs, estimates from Equation 6-10 are only +8% and -30%
8 inaccurate for naphthalene at the temperature extremes (Figure 6-5).

9 The solubility of PAHs under environmental conditions can be estimated from the following
10 relationship that is a combination of Equations 6-9 and 6-10 using the average Setschenow constant:

$$11 \quad S_{\%o} = S_0 \times 10^{-0.000583 \times \%o} \quad (6-11)$$

13
14 when %o is the salinity of the sea water. This correction for solubility can be used as part of the
15 procedures to modify this ESG for site-specific differences.

SECTION 7

SEDIMENT GUIDELINE STATEMENT

7.1 SEDIMENT GUIDELINE STATEMENT

The procedures described in this document and in the "Technical Basis for the Derivation of Equilibrium Partitioning Sediment Guidelines (ESGs) for the Protection of Benthic Organisms: Nonionic Organics" (U.S. EPA, 2000a) indicate that, except possibly where a locally important species is very sensitive or benthic organisms are exposed to both significant amounts of PAHs and UV light, benthic organisms should be acceptably protected from the effects of PAH mixtures in freshwater and saltwater sediments if the $\Sigma ESGTU_{FCV}$ is less than or equal to 1.0

$$ESG = \Sigma ESGTU = \sum_i \frac{C_{OCI}}{C_{OC,PAH,FCVi}} \leq 1.0 \quad (7-1)$$

If the $\Sigma ESGTU_{FCV}$ is equal to or less than 1.0 then the sediment meets the guideline and benthic organisms are acceptably protected from PAH mixture-induced sediment toxicity. If the $\Sigma ESGTU_{FCV}$ is greater than 1.0 the ESG for mixtures of PAHs is violated and there is reason to believe that specific sediment may be unacceptably contaminated by the mixture of PAHs.

As indicated, this sediment-specific guideline is the sum of the quotients of the concentrations of individual PAHs in a sediment, on an organic carbon basis, each divided by its respective $C_{OC,PAH,FCVi}$. At a minimum, the definition of total PAHs for this ESG requires quantification of the 34 PAHs analyzed by the U.S. EPA as part of the EMAP and REMAP programs (PAHs are identified in bold in Table 3-4) or an estimate of $\Sigma ESGTU_{FCV}$ based on the 95% uncertainty values (see Section 6.2.

1 and are compared with the compounds' concentrations at 25°C (Figure 6-5). The least-squares
2 exponential representation of the data is as follows

$$3 \quad (S_0 / {}^{25}S_0) = 0.261 \times e^{0.0536t}, r^2 = 0.959 \quad (6-10)$$

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10 relationship that is a combination of Equations 6-9 and 6-10 using the average Setschenow constant:

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Table 6-1).

The ESGs are intended to protect benthic organisms from direct toxicity associated with exposure to PAH-contaminated sediments. They are not designed to protect aquatic systems from PAH release associated, for example, with the transport of PAHs into the food web either from sediment ingestion or the ingestion of contaminated benthos.

7.2 SPECIAL CONSIDERATIONS

To establish a national guideline, certain assumptions are necessary. It is possible that site-specific conditions may affect the applicability of the national guideline. These include:

1. Fewer than 34 PAHs have been measured. Particularly in cases where historical data are being examined, chemistry data may be available for fewer than the 34 PAHs recommended for this guideline. Calculating $\Sigma\text{ESGTU}_{\text{FCV}}$ directly using fewer PAHs will generally cause the guideline to be underprotective because PAH mixtures found in the environment typically contain substantial concentrations of PAHs outside the suites of 13 or 23 PAHs commonly measured in monitoring programs. EPA has conducted an analysis of PAH distributions across many geographic regions and developed adjustment factors that can be used to adjust $\Sigma\text{ESGTU}_{\text{FCV}}$ based on subsets of 13 or 23 PAHs with varying degrees of certainty (see Section 6.2). In some applications of the PAH ESG, it may be important to minimize the frequency of false negatives (sediments judged to be acceptable when they are not). For these cases, the $\Sigma\text{ESGTU}_{\text{FCV}}$ calculated from a subset of 13 PAHs (see Table 6-2 for listing) can be multiplied by 11.5, or the $\Sigma\text{ESGTU}_{\text{FCV}}$ calculated from a subset of 23 PAHs (see Table 6-2 for listing) can be multiplied by 4.14 to achieve 95% confidence that the actual $\Sigma\text{ESGTU}_{\text{FCV}}$ for all 34 PAHs

would not be higher than the calculated value.

Use of these adjustment factors introduces uncertainty into the calculation of the $\Sigma\text{ESGTU}_{\text{FCV}}$. Consequently, a conservative estimate of the $\Sigma\text{ESGTU}_{\text{FCV}}$ is necessary, to accomplish this the uncertainty for the 95% confidence level is applied. This means that most of the sediments may contain fewer $\Sigma\text{ESGTU}_{\text{FCV}}$ than indicated by the calculation. In cases where less conservative assumptions are appropriate, factors with lower confidence can be applied, as detailed in Section 6.2. In any case, avoiding the uncertainty introduced by the use of adjustment factors is the primary reason EPA recommends that wherever possible, a more complete PAH analysis is undertaken. In cases where adjustment factors are used and the calculated $\Sigma\text{ESGTU}_{\text{FCV}}$ are greater than the ESG, it may be particularly advantageous to eliminate the uncertainty by conducting additional analyses.

2. **Interaction of PAHs with UV light.** Guidelines calculated in this document are based on narcotic toxicity only and do not consider enhanced toxicity that can occur if PAH-exposed organisms are simultaneously exposed to UV light. In environments where significant sunlight penetrates to the sediment and benthic organisms are exposed to UV light, the ESG may be underprotective. Consult Section 6.4 for additional details.
3. **Influence of soot and coal on PAH partitioning.** Literature data have indicated that soot and/or coal particles in sediment may contain PAHs that partition less to interstitial water than those associated with typical organic carbon, thereby causing the guideline to be overprotective. The influence of these phases can be assessed by measuring concentrations of PAHs directly in interstitial water and comparing these measures with concentrations predicted

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1 by EqP. See Section 6.7 and the site-specific ESG guidelines (U.S. EPA, 2000f) for further
2 discussion.

3
4 4. **Unusual composition of organic carbon.** Partition coefficients used for calculating the
5 national PAH mixture ESG are based on measured partitioning from natural organic carbon in
6 typical field sediments. Some sediments influenced heavily by industrial activities may contain
7 sources of organic carbon whose partitioning properties are not similar, such as rubber, animal
8 processing wastes (e.g., hair or hide fragments), or wood processing wastes (bark, wood fiber
9 or chips). Relatively undegraded woody debris or plant matter (e.g., roots, leaves) may also
10 contribute organic carbon that results in partitioning different from that of typical organic
11 carbon. Sediments with large amounts of these materials may show higher concentrations of
12 chemicals in interstitial water than would be predicted using generic K_{oc} values, making the
13 ESG underprotective. Direct analysis of interstitial water can be used to evaluate this
14 possibility (see U.S. EPA, 2000a,f).

15
16 5. **Presence of additional narcotic compounds.** The PAH mixture ESG is based on the
17 additivity of non-polar narcotic toxicants, such as PAHs. However, some sediments may
18 contain additional compounds that would contribute to narcotic toxicity, such as chlorobenzenes
19 or PCBs (note: PCBs may also cause adverse effects through bioaccumulation and transfer to
20 higher trophic levels; these bioaccumulative effects are not addressed by this narcosis-based
21 ESG and should be evaluated separately). The presence of additional non-polar narcotic
22 chemicals may make the PAH mixture ESG underprotective, because the ESG itself only
23 addresses that part of the narcotic potency caused by PAHs. Di Toro et al. (2000) and Di Toro
24 and McGrath, 2000) describe methods by which the contributions of other narcotic chemicals

1 can be incorporated into an ESG-type assessment.

2
3 6. **Site-specific temperature and salinity corrections.** Temperature and salinity both affect
4 solubility of PAHs and can therefore affect the solubility-constrained maximum contribution of
5 individual PAHs to the overall ESG. Solubilities used in this document are calculated for 25°C
6 and salinity less than 1‰. Solubilities can be recalculated to meet site specific conditions
7 using procedures described in Section 6.8. Within a range of 0 to 35°C and salinity from 0 to
8 35‰, solubility can be expected to decrease by a factor of about 30 to 40% with decrease in
9 temperature or increase in salinity. Site-specific recalculation of solubilities will only affect
10 $\Sigma\text{ESGTU}_{\text{FCV}}$ in cases where the contribution of one or more PAHs are solubility constrained
11 (see Section 6.8).

1 by EqP. See Section 6.7 and the site-specific ESG guidelines (U.S. EPA, 2000f) for further
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7 using procedures described in Section 6.8. Within a range of 0 to 35°C and salinity from 0 to
8 35‰, solubility can be expected to decrease by a factor of about 30 to 40% with decrease in
9 temperature or increase in salinity. Site-specific recalculation of solubilities will only affect
10 $\Sigma\text{ESGTU}_{\text{PCV}}$ in cases where the contribution of one or more PAHs are solubility constrained
11 (see Section 6.8).

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Table 2-1. Regression results: y-intercepts and chemical class corrections[†] (Table from Di Toro et al., 2000).

Species <i>i</i>	<i>N</i>	<i>b_i</i>	<i>SE(b_i)</i>	10^{b_i}	<i>SE</i> (10^{b_i})
				$\mu\text{mol/g octanol}$	
<i>Americamysis bahia</i>	30	1.54	0.082	34.3	6.7
<i>Portunus pelagicus</i>	4	1.56	0.190	36.1	18.2
<i>Leptocheirus plumulosus</i>	4	1.56	0.191	36.2	18.4
<i>Palaemonetes pugio</i>	8	1.68	0.137	48.2	16.4
<i>Oncorhynchus mykiss</i>	44	1.79	0.065	61.7	9.4
<i>Jordanella floridae</i>	18	1.82	0.096	66.1	15.2
<i>Ictalurus punctatus</i>	7	1.87	0.139	74.8	25.9
<i>Pimephales promelas</i>	182	2.02	0.044	105	10.8
<i>Lepomis macrochirus</i>	70	2.03	0.0056	108	14.1
<i>Daphnia magna</i>	113	2.04	0.049	111	12.6
<i>Cyprinodon variegatus</i>	33	2.05	0.078	111	20.5
<i>Oryzias latipes</i>	4	2.05	0.182	112	53.9
<i>Carassius auratus</i>	43	2.13	0.065	134	20.5
<i>Rana catesbeian</i>	5	2.13	0.162	135	55.9
<i>Tarystarsus dissimilis</i>	9	2.14	0.125	137	42.0
<i>Orconectes immunis</i>	6	2.14	0.149	139	52.3
<i>Alburnus alburnus</i>	7	2.16	0.137	144	49.1
<i>Nitocra spinipes</i>	6	2.17	0.148	147	54.7
<i>Gambusia affinis</i>	8	2.17	0.130	149	47.9
<i>Leucisus idus melanotus</i>	26	2.18	0.075	152	26.8
<i>Neanthes arenaceodentata</i>	4	2.23	0.19	168	85
<i>Artemia salina nauplii</i>	32	2.26	0.077	181	32.8
<i>Lymnaea stagnalis</i>	5	2.29	0.163	195	81.5
<i>Xenopus laevis</i>	5	2.33	0.163	213	88.9
<i>Hydra oligactis</i>	5	2.33	0.163	214	89.5
<i>Culex pipiens</i>	5	2.34	0.163	216	90.4
<i>Poecilia reticulata</i>	14	2.36	0.101	228	55.2
<i>Menidia beryllina</i>	8	2.37	0.134	233	77.3

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Table 2-1. Regression results: y-intercepts and chemical class corrections[†] (Table from Di Toro et al., 2000).

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<i>Pimephales promelas</i>	182	2.02	0.044	105	10.8
<i>Lepomis macrochirus</i>	70	2.03	0.0056	108	14.1
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Species <i>i</i>	<i>N</i>	<i>b_i</i>	<i>SE(b_i)</i>	10^{b_i}	<i>SE</i> (10^{b_i})
				$\mu\text{mol/g octanol}$	
<i>Daphnia pulex</i>	6	2.38	0.150	240	91
<i>Ambystoma mexicanum</i>	5	2.39	0.163	245	103
<i>Daphnia cucullata</i>	5	2.4	0.163	249	104
<i>Aedes aegypti</i>	5	2.42	0.163	261	109
<i>Tetrahymena ellioti</i>	10	2.46	0.121	286	85
Chemical Class <i>l</i>	<i>N</i>	Δc_l	<i>SE</i> (Δc_l)	$10^{\Delta c_l}$	<i>SE</i> ($10^{\Delta c_l}$)
Aliphatics	215	0.00	-	1.0	-
Ethers	13	0.00	-	1.0	-
Alcohols	134	0.00	-	1.0	-
Aromatics	241	0.00	-	1.0	-
Halogenated	319	-0.244	0.033	0.570	0.044
Ketones	49	-0.245	0.059	0.569	0.078
PAHs	84	-0.263	0.057	0.546	0.073
Slope		-0.945	0.014		

[‡]See Equation (2-7).

N = Number of data points.

b_i = y-intercept.

SE(b_i) = Standard error of *b_i*.

Δc_l = chemical class correction to the y-intercept.

SE(Δc_l) = standard error of Δc_l .

[†] = Standard errors of 10^{b_i} and $10^{\Delta c_l}$ are based on the assumption that the estimation errors for *b_i* and Δc_l are gaussian. The formulas follow from the standard error of a log normally distributed random variable (Aitchison and Brown, 1957). For $x = b_i$ or Δc_l , $\mu_x = 2.303x$, $\sigma_x = 2.303 \times SE(x)$, and

$$SE(10^x) = SE(e^{2.303x}) = e^{\mu_x} \sqrt{e^{2\sigma_x^2} - e^{2\sigma_x^2}}$$

Table 2-2. Comparison of body burdens observed in aquatic organisms acutely exposed to narcotic chemicals and body burdens predicted from target lipid narcosis theory (Table from Di Toro et al., 2000).

Organism	Chemical	log K_{OW}	time hr	C_{ORG}		References
				Obs	Pred.	
				$\mu\text{mol}/\text{g lipid}$	$\mu\text{mol}/\text{g octanol}$	
Mosquitofish, <i>Gambusia affinis</i>	1,4-dibromobenzene	3.55	96	85.0		Chaisuksant and Connell, 1997
	1,2,3-trichlorobenzene	3.98	"	140.0		
	1,2,4-trichlorobenzene	4.00	"	92.0		
	pentachlorobenzene	5.32	"	69.0	93.2 85.3	
Guppy, <i>Poecilia reticulata</i>	1,4-difluorobenzene	2.11	1.5	444.0		Sijm et al., 1993
	1,2-dichlorobenzene	3.31	91	34.0		
	1,4-dichlorobenzene	3.24	41	400.0		
	1,2-dibromobenzene	3.56	4	24.0		
	1,4-dibromobenzene	3.55	60	120.0	110.0 130.0	
Fathead minnow, <i>Pimephales promelas</i>	1,2-dichlorobenzene	3.31	18	78.0		Sijm et al., 1993
	1,4-dichlorobenzene	3.24	10	68.0		
	1,2-dibromobenzene	3.56	7	60.0		
	1,4-dibromobenzene	3.55	10	54.0		
Fathead minnow, <i>Pimephales promelas</i>	1,2,4-trichlorobenzene	4.00	50.2			van Wezel et al., 1995
	1,1,2,2-tetrachlorobenzene	2.31	57.2			
	dichlorobenzene	3.27	75.5			
	dichlorobenzene	3.27	129			
	1,2-dichlorobenzene	3.31	62.3			
Fathead minnow, <i>Pimephales promelas</i>	1,2-dichlorobenzene	3.31		98.9		van Wezel et al., 1996
	1,4-dichlorobenzene	3.24		173		
	1,4-dichlorobenzene	3.24		121		
	1,2 + 1,4-dichlorobenzene			107		
	1,2 + 1,4-dichlorobenzene			110		
	1,2 + 1,4-dichlorobenzene			138		
	1,2 + 1,4-dichlorobenzene			150		
Fathead minnow, <i>Pimephales promelas</i>	naphthalene	3.36		123	95.0 59.9	de Maagd et al., 1996
	1,2,4-trichlorobenzene	4.00		215		

Species <i>i</i>	<i>N</i>	<i>b_i</i>	<i>SE(b_i)</i>	10^{b_i}	<i>SE</i> (10^{b_i})
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Ethers	13	0.00	-	1.0	-
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Halogenated	319	-0.244	0.033	0.570	0.044
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PAHs	84	-0.263	0.057	0.546	0.073
Slope		-0.945	0.014		

^aSee Equation (2-7).

N = Number of data points.

b_i = *y*-intercept.

SE(*b_i*) = Standard error of *b_i*.

Δc_l = chemical class correction to the *y*-intercept.

SE(Δc_l) = standard error of Δc_l .

[†] = Standard errors of 10^{b_i} and $10^{\Delta c_l}$ are based on the assumption that the estimation errors for *b_i* and Δc_l are gaussian. The formulas follow from the standard error of a log normally distributed random variable (Aitchison and Brown, 1957). For *x* = *b_i* or Δc_l , $\mu_t = 2.303x$, $\sigma_t = 2.303 \times SE(x)$, and

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Organism	Chemical	log K_{OW}	time hr	C_{ORG}		References
				Obs	Pred.	
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	1,2,3-trichlorobenzene	3.98	"	140.0		
	1,2,4-trichlorobenzene	4.00	"	92.0		
	pentachlorobenzene	5.32	"	69.0	93.2 85.3	
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	1,2-dichlorobenzene	3.31	91	34.0		
	1,4-dichlorobenzene	3.24	41	400.0		
	1,2-dibromobenzene	3.56	4	24.0		
	1,4-dibromobenzene	3.55	60	120.0	110.0 130.0	
Fathead minnow, <i>Pimephales promelas</i>	1,2-dichlorobenzene	3.31	18	78.0		Sijm et al., 1993
	1,4-dichlorobenzene	3.24	10	68.0		
	1,2-dibromobenzene	3.56	7	60.0		
	1,4-dibromobenzene	3.55	10	54.0		
Fathead minnow, <i>Pimephales promelas</i>	1,2,4-trichlorobenzene	4.00	50.2			van Wezel et al., 1995
	1,1,2,2-tetrachlorobenzene	2.31	57.2			
	dichlorobenzene	3.27	75.5			
	dichlorobenzene	3.27	129			
	1,2-dichlorobenzene	3.31	62.3			
Fathead minnow, <i>Pimephales promelas</i>	1,2-dichlorobenzene	3.31		98.9		van Wezel et al., 1996
	1,4-dichlorobenzene	3.24		173		
	1,4-dichlorobenzene	3.24		121		
	1,2 + 1,4-dichlorobenzene			107		
	1,2 + 1,4-dichlorobenzene			110		
	1,2 + 1,4-dichlorobenzene			138		
	1,2 + 1,4-dichlorobenzene			150		
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Organism	Chemical	log <i>K</i> _{ow}	time hr	<i>C</i> _{org}			References
				Obs	Mean	Pred.	
					μmol/ g lipid	μmol/ g octanol	
Amphipod, <i>Leptocheirus plumulosus</i>	Fluoranthene	5.08	24	14.0	26.1	19.8	Driscoll, S.K. and L.C. Schaffner, 1997
	Fluoranthene	5.08	24	48.8			
<hr/>							
Crab, <i>Portunus pelagicus</i>	1,4-dichlorobenzene	3.24	96	9.6			Mortimer and Connell, 1994
	1,2,3-trichlorobenzene	3.98	96	45.0			
	1,2,3,4-tetrachlorobenzene	4.64	96	119			
	pentachlorobenzene	5.32	96	111	49.9	20.6	

Table 3-1. Summary of the chronic sensitivity of freshwater and saltwater organisms to PAHs; test-specific data.

Common Name, Species Name	Test ^a	Habitat ^b	PAH tested	Duration	NOEC ($\mu\text{g/L}$)	OEC ($\mu\text{g/L}$)	Observed Effects (Relative to Controls)	Chronic Value ($\mu\text{g/L}$)	Reference
Cladoceran, <i>Daphnia magna</i>	LC	W	Anthracene	21d		2.1	5.3% fewer broods	<2.1	Holst and Giesy, 1989
						4.0	8.0% fewer broods		
						8.2	13.8% fewer broods		
Cladoceran, <i>Daphnia magna</i>	LC	W	Fluoranthene	21d	6.9-17	35	17% reduction in length	24.5	Spehar et al., 1999
						73	25% reduction in length, 37% fewer young/adult		
						148	No survival		
Cladoceran, <i>Daphnia magna</i>	LC	W	Phenanthrene	21d	46-57	163	Survival reduced 83%, 98% fewer broods	96.39	Call et al., 1986
Midge, <i>Paratanytarsus sp.</i>	LC	B	Acenaphthene	26d	32-295	575	Survival reduced ~90%, ~60% reduction in growth, no reproduction	411.8	Northwestern Aquatic Sciences, 1982
Midge, <i>Paratanytarsus sp.</i>	LC	B	Acenaphthene	26d	27-164	315	Survival reduced ~20%, ~30% reduction in growth	227.3	Northwestern Aquatic Sciences, 1982; Thursby, 1991a

Organism	Chemical	log K_{ow}	time hr	C_{org}			References
				Obs	Mean	Pred.	
					$\mu\text{mol}/\text{g lipid}$	$\mu\text{mol}/\text{g octanol}$	
Amphipod, <i>Leptocheirus plumulosus</i>	Fluoranthene	5.08	24	14.0	26.1	19.8	Driscoll, S.K. and L.C. Schaffner, 1997
	Fluoranthene	5.08	24	48.8			
Crab, <i>Portunus pelagicus</i>	1,4-dichlorobenzene	3.24	96	9.6			Mortimer and Connell, 1994
	1,2,3-trichlorobenzene	3.98	96	45.0			
	1,2,3,4-tetrachlorobenzene	4.64	96	119			
	pentachlorobenzene	5.32	96	111	49.9	20.6	

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Common Name, Species Name	Test ^a	Habitat ^b	PAH tested	Duration	NOEC ($\mu\text{g/L}$)	OEC ($\mu\text{g/L}$)	Observed Effects (Relative to Controls)	Chronic Value ($\mu\text{g/L}$)	Reference
Cladoceran, <i>Daphnia magna</i>	LC	W	Anthracene	21d		2.1	5.3% fewer broods	<2.1	Hoist and Giesy, 1989
						4.0	8.0% fewer broods		
						8.2	13.8% fewer broods		
Cladoceran, <i>Daphnia magna</i>	LC	W	Fluoranthene	21d	6.9-17	35	17% reduction in length	24.5	Spehar et al., 1999
						73	25% reduction in length, 37% fewer young/adult		
						148	No survival		
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Midge, <i>Paratanytarsus sp.</i>	LC	B	Acenaphthene	26d	27-164	315	Survival reduced ~20%, ~30% reduction in growth	227.3	Northwestern Aquatic Sciences, 1982; Thursby, 1991a

Common Name, Species Name	Test ^a	Habitat ^b	PAH tested	Duration	NOEC (µg/L)	OEC (µg/L)	Observed Effects (Relative to Controls)	Chronic Value (µg/L)	Reference
						676	Survival reduced ~60%		
Fathead minnow, <i>Pimephales promelas</i>	ELS	W	Acenaphthene	32d	50	109	5% reduction in growth	73.82	Academy of Natural Sciences, 1981; Thursby, 1991a
						410	26% reduction in growth, Survival reduced 45%		
						630	No survival		
Fathead minnow, <i>Pimephales promelas</i>	ELS	W	Acenaphthene	32d	50-109	410	20% reduction in growth, Survival reduced 66%	211.4	Academy of Natural Sciences, 1981; Thursby, 1991a
						630	No survival		
Fathead minnow, <i>Pimephales promelas</i>	ELS	W	Acenaphthene	32-35d	67-332	495	54% reduction in growth	405.4	Cairns and Nebeker, 1982
Fathead minnow, <i>Pimephales promelas</i>	ELS	W	Acenaphthene	32-35d	197-345	509	30% reduction in growth	419.0	Cairns and Nebeker, 1982
						682	52% reduction in growth, Survival reduced 45%		
						1153	87% reduction in growth, Survival reduced 97%		

Common Name, <i>Species Name</i>	Test ^a	Habitat ^b	PAH tested	Duration	NOEC ($\mu\text{g/L}$)	OEC ($\mu\text{g/L}$)	Observed Effects (Relative to Controls)	Chronic Value ($\mu\text{g/L}$)	Reference
Fathead minnow, <i>Pimephales promelas</i>	ELS	W	Acenaphthene	32d	64	98	Survival reduced 24%	79.20	ERCO, 1981
						149	Survival reduced 65%		
						271	Survival reduced 75%		
						441	Survival reduced 80%		
Fathead minnow, <i>Pimephales promelas</i>	ELS	W	Acenaphthene	32d	50-91	139	Survival reduced 20%	112.5	ERCO, 1981
						290	Survival reduced 50%		
						426	Survival reduced 52%		
Fathead minnow, <i>Pimephales promelas</i>	ELS	W	Fluoranthene	32d	3.7-10.4	21.7	Survival reduced 67%, 50% reduction in growth	15.02	Spehar et al., 1999
Rainbow trout, <i>Oncorhynchus mykiss</i>	ELS	B/W	Phenanthrene	90d	5	8	Survival reduced 41%, 33% reduced growth	6.325	Call et al., 1986
						14	Survival reduced 48%, 44% reduced growth		
						32	Survival reduced 52%, 75% reduced growth		
						66	No survival		

Common Name, Species Name	Test ^a	Habitat ^b	PAH tested	Duration	NOEC ($\mu\text{g/L}$)	OEC ($\mu\text{g/L}$)	Observed Effects (Relative to Controls)	Chronic Value ($\mu\text{g/L}$)	Reference
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						630	No survival		
Fathead minnow, <i>Pimephales promelas</i>	ELS	W	Acenaphthene	32-35d	67-332	495	54% reduction in growth	405.4	Cairns and Nebeker, 1982
Fathead minnow, <i>Pimephales promelas</i>	ELS	W	Acenaphthene	32-35d	197-345	509	30% reduction in growth	419.0	Cairns and Nebeker, 1982
						682	52% reduction in growth, Survival reduced 45%		
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Common Name, <i>Species Name</i>	Test ^a	Habitat ^b	PAH tested	Duration	NOEC ($\mu\text{g/L}$)	OEC ($\mu\text{g/L}$)	Observed Effects (Relative to Controls)	Chronic Value ($\mu\text{g/L}$)	Reference
Fathead minnow, <i>Pimephales promelas</i>	ELS	W	Acenaphthene	32d	64	98	Survival reduced 24%	79.20	ERCO, 1981
						149	Survival reduced 65%		
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Fathead minnow, <i>Pimephales promelas</i>	ELS	W	Acenaphthene	32d	50-91	139	Survival reduced 20%	112.5	ERCO, 1981
						290	Survival reduced 50%		
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Rainbow trout, <i>Oncorhynchus mykiss</i>	ELS	B/W	Phenanthrene	90d	5	8	Survival reduced 41%, 33% reduced growth	6.325	Call et al., 1986
						14	Survival reduced 48%, 44% reduced growth		
						32	Survival reduced 52%, 75% reduced growth		
						66	No survival		

Common Name, <i>Species Name</i>	Test ^a	Habitat ^b	PAH tested	Duration	NOEC ($\mu\text{g/L}$)	OEC ($\mu\text{g/L}$)	Observed Effects (Relative to Controls)	Chronic Value ($\mu\text{g/L}$)	Reference
Mysid, <i>Americamysis bahia</i>	LC	B/W	Acenaphthene	35d	100-240	340	93% reduction in young	285.7	Horne et al., 1983
						510	No survival		
Mysid, <i>Americamysis bahia</i>	LC	B/W	Acenaphthene	25d	20.5-44.6	91.8	91% reduction in young	63.99	Thursby et al., 1989b
						168	No reproduction, 34% reduction in growth		
						354	Survival reduced 96%, no reproduction		
Mysid, <i>Americamysis bahia</i>	LC	B/W	Fluoranthene	28d	5-12	21	Survival reduced 26.7%, 91.7% reduction in young	15.87	U.S. EPA, 1978
						43	No survival		
Mysid, <i>Americamysis bahia</i>	LC	B/W	Fluoranthene	31d	0.41-11.1	18.8	Survival reduced 23%, no reproduction	14.44	Spehar et al., 1999
Mysid, <i>Americamysis bahia</i>	LC	B/W	Phenanthrene	32d	1.5-5.5	11.9	No survival	8.129	Kuhn and Lussier, 1987
Mysid, <i>Americamysis bahia</i>	LC	B/W	Pyrene	28d	3.82	5.37	46% reduction in young	4.53	Champlin and Poucher, 1992c
						6.97	47% reduction in young		

Common Name, Species Name	Test ^a	Habitat ^b	PAH tested	Duration	NOEC ($\mu\text{g/L}$)	OEC ($\mu\text{g/L}$)	Observed Effects (Relative to Controls)	Chronic Value ($\mu\text{g/L}$)	Reference
						9.82	73% reduction in young		
						15.8	85% reduction in young		
						20.9	90% reduction in young, Survival reduced 37%		
						38.2	No survival		
Sheepshead minnow, <i>Cyprinodon variegatus</i>	ELS	B/W	Acenaphthene	28d	240-520	970	Survival reduced 70%	710.2	Ward et al., 1981
						2000	No survival		
						2800	No survival		

^a TEST: LC = life-cycle, PLC = partial life-cycle, ELS = early life-stage

^b HABITAT: I = infauna, E = epibenthic, W = water column

^c NOEC = Concentrations where no significant effects were detected.

^d OEC = Concentrations where significant effects were detected on survival, growth, or reproduction.

Common Name, <i>Species Name</i>	Test ^a	Habitat ^b	PAH tested	Duration	NOEC ($\mu\text{g/L}$)	OE ($\mu\text{g/L}$)	Observed Effects (Relative to Controls)	Chronic Value ($\mu\text{g/L}$)	Reference
Mysid, <i>Americamysis bahia</i>	LC	B/W	Acenaphthene	35d	100-240	340	93% reduction in young	285.7	Horne et al., 1983
						510	No survival		
Mysid, <i>Americamysis bahia</i>	LC	B/W	Acenaphthene	25d	20.5-44.6	91.8	91% reduction in young	63.99	Thursby et al., 1989b
						168	No reproduction, 34% reduction in growth		
						354	Survival reduced 96%, no reproduction		
Mysid, <i>Americamysis bahia</i>	LC	B/W	Fluoranthene	28d	5-12	21	Survival reduced 26.7%, 91.7% reduction in young	15.87	U.S. EPA, 1978
						43	No survival		
Mysid, <i>Americamysis bahia</i>	LC	B/W	Fluoranthene	31d	0.41-11.1	18.8	Survival reduced 23%, no reproduction	14.44	Spehar et al., 1999
Mysid, <i>Americamysis bahia</i>	LC	B/W	Phenanthrene	32d	1.5-5.5	11.9	No survival	8.129	Kuhn and Lussier, 1987
Mysid, <i>Americamysis bahia</i>	LC	B/W	Pyrene	28d	3.82	5.37	46% reduction in young	4.53	*Champlin and Poucher, 1992c
						6.97	47% reduction in young		

Common Name, Species Name	Test ^a	Habitat ^b	PAH tested	Duration	NOEC (µg/L)	OEC (µg/L)	Observed Effects (Relative to Controls)	Chronic Value (µg/L)	Reference
						9.82	73% reduction in young		
						15.8	85% reduction in young		
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Sheepshead minnow, <i>Cyprinodon variegatus</i>	ELS	B/W	Acenaphthene	28d	240-520	970	Survival reduced 70%	710.2	Ward et al., 1981
						2000	No survival		
						2800	No survival		

^a TEST: LC = life-cycle, PLC = partial life-cycle, ELS = early life-stage

^b HABITAT: I = infauna, E = epibenthic, W = water column

^c NOEC = Concentrations where no significant effects were detected.

^d OEC = Concentrations where significant effects were detected on survival, growth, or reproduction.

Table 3-2. Acute and chronic values, acute-chronic ratios and derivation of the final acute values, final acute-chronic values and final chronic values.

Common Name, Scientific name	PAH Tested	Acute Value μg/L	Chronic Value μg/L	Acute- Chronic Ratio	PAH-Specific Mean Acute- Chronic Ratio	Species Mean Acute- Chronic Ratio	Reference
<u>FRESHWATER SPECIES</u>							
Cladoceran, <i>Daphnia magna</i>	Anthracene	-	<2.1	-	-	-	Holst and Giesy, 1989
Cladoceran, <i>Daphnia magna</i>	Fluoranthene	117	24.5	4.78	4.78	-	Spehar et al., 1999
Cladoceran, <i>Daphnia magna</i>	Phenanthrene	117	96.4	1.21	1.21	2.41	Call et al., 1986
Midge, <i>Paratanytarsus</i> sp.	Acenaphthene	2,040 ^a	411	4.96	-	-	Northwestern Aquatic Sciences, 1982
Midge, <i>Paratanytarsus</i> sp.	Acenaphthene	2,040 ^a	227	9.00	6.68	6.68	Northwestern Aquatic Sciences, 1982; Thursby, 1991a
Fathead Minnow, <i>Pimephales promelas</i>	Acenaphthene	608	405	1.50	-	-	Cairns and Nebeker, 1982; Thursby, 1991a
Fathead Minnow, <i>Pimephales promelas</i>	Acenaphthene	608	419	1.45	1.4	-	Cairns and Nebeker, 1982
Fathead Minnow, <i>Pimephales promelas</i>	Acenaphthene	-	73.82	-	-	-	Academy of Natural Sciences, 1981
Fathead Minnow, <i>Pimephales promelas</i>	Acenaphthene	-	211	-	-	-	Academy of Natural Sciences, 1981
Fathead Minnow, <i>Pimephales promelas</i>	Acenaphthene	-	79.2	-	-	-	ERCO, 1981
Fathead Minnow, <i>Pimephales promelas</i>	Acenaphthene	-	112	-	-	-	ERCO, 1981
Fathead Minnow, <i>Pimephales promelas</i>	Fluoranthene	69 ^c	15.0	4.60	4.60	2.61	Spehar et al., 1999

Common Name, Scientific name	PAH Tested	Acute Value $\mu\text{g/L}$	Chronic Value $\mu\text{g/L}$	Acute- Chronic Ratio	PAH-Specific Mean Acute- Chronic Ratio	Species Mean Acute- Chronic Ratio	Reference
Rainbow trout, <i>Oncorhynchus mykiss</i>	Phenanthrene	50 ^c	6.32	7.90	7.90	7.90	Call et al., 1986
<u>SALTWATER SPECIES</u>							
Mysid, <i>Americamysis bahia</i>	Acenaphthene	466	286	1.63	-	-	Horne et al., 1983
Mysid, <i>Americamysis bahia</i>	Acenaphthene	460	64.0	7.19	3.42	-	Thursby et al., 1989b
Mysid, <i>Americamysis bahia</i>	Fluoranthene	40	15.9	2.52	-	-	U.S. EPA, 1978
Mysid, <i>Americamysis bahia</i>	Fluoranthene	31	14.4	2.15	2.33	-	Spehar et al., 1999
Mysid, <i>Americamysis bahia</i>	Phenanthrene	27.1	8.13	3.33	3.33	-	Kuhn and Lussier, 1987
Mysid, <i>Americamysis bahia</i>	Pyrene	28.3	4.53	6.24	6.24	3.59	Champlin and Poucher, 1992c
Sheepshead minnow, <i>Cyprinodon variegatus</i>	Acenaphthene	3,100 ^b	710	4.37	4.37	4.37	Ward et al., 1981

^a Geometric mean of two flow-through measured tests from the same laboratory as conducted the life-cycle tests.

^b LC50 concentration slightly greater than acenaphthene's water solubility.

^c EC50 based on immobilization used as the acute value instead of the LC50.

Final Acute Value = 9.32 $\mu\text{mol/g}$ octanol

Final Acute-chronic Ratio = 4.16

Final Chronic Value = 2.24 $\mu\text{mol/g}$ octanol

Table 3-2. Acute and chronic values, acute-chronic ratios and derivation of the final acute values, final acute-chronic values and final chronic values.

Common Name, Scientific name	PAH Tested	Acute Value µg/L	Chronic Value µg/L	Acute- Chronic Ratio	PAH-Specific Mean Acute- Chronic Ratio	Species Mean Acute- Chronic Ratio	Reference
<u>FRESHWATER SPECIES</u>							
Cladoceran, <i>Daphnia magna</i>	Anthracene	-	<2.1	-	-	-	Holst and Giesy, 1989
Cladoceran, <i>Daphnia magna</i>	Fluoranthene	117	24.5	4.78	4.78	-	Spehar et al., 1999
Cladoceran, <i>Daphnia magna</i>	Phenanthrene	117	96.4	1.21	1.21	2.41	Call et al., 1986
Midge, <i>Paratanytarsus</i> sp.	Acenaphthene	2,040 ^a	411	4.96	-	-	Northwestern Aquatic Sciences, 1982
Midge, <i>Paratanytarsus</i> sp.	Acenaphthene	2,040 ^a	227	9.00	6.68	6.68	Northwestern Aquatic Sciences, 1982; Thursby, 1991a
Fathead Minnow, <i>Pimephales promelas</i>	Acenaphthene	608	405	1.50	-	-	Cairns and Nebeker, 1982; Thursby, 1991a
Fathead Minnow, <i>Pimephales promelas</i>	Acenaphthene	608	419	1.45	1.4	-	Cairns and Nebeker, 1982
Fathead Minnow, <i>Pimephales promelas</i>	Acenaphthene	-	73.82	-	-	-	Academy of Natural Sciences, 1981
Fathead Minnow, <i>Pimephales promelas</i>	Acenaphthene	-	211	-	-	-	Academy of Natural Sciences, 1981
Fathead Minnow, <i>Pimephales promelas</i>	Acenaphthene	-	79.2	-	-	-	ERCO, 1981
Fathead Minnow, <i>Pimephales promelas</i>	Acenaphthene	-	112	-	-	-	ERCO, 1981
Fathead Minnow, <i>Pimephales promelas</i>	Fluoranthene	69 ^c	15.0	4.60	4.60	2.61	Spehar et al., 1999

Common Name, Scientific name	PAH Tested	Acute Value μg/L	Chronic Value μg/L	Acute- Chronic Ratio	PAH-Specific Mean Acute- Chronic Ratio	Species Mean Acute- Chronic Ratio	Reference
Rainbow trout, <i>Oncorhynchus mykiss</i>	Phenanthrene	50 ^c	6.32	7.90	7.90	7.90	Call et al., 1986
<u>SALTWATER SPECIES</u>							
Mysid, <i>Americamysis bahia</i>	Acenaphthene	466	286	1.63	-	-	Horne et al., 1983
Mysid, <i>Americamysis bahia</i>	Acenaphthene	460	64.0	7.19	3.42	-	Thursby et al., 1989b
Mysid, <i>Americamysis bahia</i>	Fluoranthene	40	15.9	2.52	-	-	U.S. EPA, 1978
Mysid, <i>Americamysis bahia</i>	Fluoranthene	31	14.4	2.15	2.33	-	Spehar et al., 1999
Mysid, <i>Americamysis bahia</i>	Phenanthrene	27.1	8.13	3.33	3.33	-	Kuhn and Lussier, 1987
Mysid, <i>Americamysis bahia</i>	Pyrene	28.3	4.53	6.24	6.24	3.59	Champlin and Poucher, 1992c
Sheepshead minnow, <i>Cyprinodon variegatus</i>	Acenaphthene	3,100 ^b	710	4.37	4.37	4.37	Ward et al., 1981

^a Geometric mean of two flow-through measured tests from the same laboratory as conducted the life-cycle tests.

^b LC50 concentration slightly greater than acenaphthene's water solubility.

^c EC50 based on immobilization used as the acute value instead of the LC50.

Final Acute Value = 9.32 μmol/g octanol

Final Acute-chronic Ratio = 4.16

Final Chronic Value = 2.24 μmol/g octanol

Table 3-3. Results of approximate randomization (AR) test for the equality of the freshwater and saltwater FAV distributions at a K_{ow} of 1.0 and AR test for the equality of benthic and combined benthic and water column FAVs for freshwater and saltwater distributions.

Comparison	Habitat or Water Type ^A		AR Statistic ^B	Probability ^C
Fresh vs Salt	Fresh (20)	Salt (29)	5.746	93.5
Freshwater: Benthic vs WQC ^D	WQC (49)	Benthic (33)	0.862	82.8

^AValues in parantheses are the number of GMAVS at a K_{ow} of 1.0 used in the comparison.

^BAR statistic = FAV difference between original compared groups.

^CProbability that the theoretical AR statistic \leq the observed AR statistic given that all samples came from the same population.

^DCombined Freshwater and Saltwater.

Table 3-4. $C_{OC,PAH,FCV}$ concentrations at a K_{OW} of 1.0 and properties required for their derivation^A.

PAH ^B	CAS # ^C	Molecular Weight ($\mu\text{g}/\mu\text{mol}$)	Mackay Solid Solubility ^D ($\mu\text{g}/\text{L}$)	SPARC ^E $\log_{10}K_{OW}$	$\log_{10}K_{OC}$	FCV ($\mu\text{mol}/\text{g octanol}$)	PAH specific FCV ($\mu\text{mol}/\text{L}$)	PAH specific FCV ($\mu\text{g}/\text{L}$)	$C_{OC,PAH,FCV}$ ($\mu\text{g}/\text{goc}$)	$C_{OC,PAH,Mari}$ ^F ($\mu\text{g}/\text{goc}$)
indan	496117	118.18	100000	3.158	3.105	2.240	2.322	274.5	349	127200
naphthalene	91203	128.17	30995	3.356	3.299	2.240	1.509	193.5	385	61700
C1-naphthalenes	-	142.20	??	3.800	3.736	2.240	0.5744	81.69	444	-
1-methylnaphthalene	90120	142.20	28001	3.837	3.772	2.240	0.5300	75.37	446	165700
2-methylnaphthalene	91576	142.20	25000	3.857	3.792	2.240	0.5074	72.16	447	154800
acnaphthylene	208968	152.2	16314	3.223	3.168	2.240	2.016	306.9	452	24000
acenaphthene	83329	154.21	3800	4.012	3.944	2.240	0.3622	55.85	491	33400
1-ethylnaphthalene	1127760	156.23	10100	4.221	4.150	2.240	0.2298	35.91	507	142500
2-ethylnaphthalene	939275	156.23	8001	4.283	4.210	2.240	0.2008	31.37	509	129900
C2-naphthalenes	-	156.23	??	4.300	4.227	2.240	0.1935	30.24	510	-
1,4-dimethylnaphthalene	571584	156.23	11400	4.300	4.227	2.240	0.1935	30.24	510	192300
1,3-dimethylnaphthalene	575417	156.23	8001	4.367	4.293	2.240	0.1673	26.13	513	157100
2,6-dimethylnaphthalene	581420	156.23	1700	4.373	4.299	2.240	0.1651	25.79	513	33800
2,3-dimethylnaphthalene	581408	156.23	2500	4.374	4.300	2.240	0.1647	25.74	513	49900
1,5-dimethylnaphthalene	571619	156.23	3100	4.378	4.304	2.240	0.1633	25.52	514	62400
fluorene	86737	166.22	1900	4.208	4.137	2.240	0.2364	39.30	538	26000
C3-naphthalenes	-	170.25	??	4.800	4.719	2.240	0.06520	11.10	581	-
2,3,5-trimethylnaphthalene	2245387	170.26	??	4.858	4.776	2.240	0.05747	9.785	584	-
1,4,5-trimethylnaphthalene	213411	170.2	2100	4.872	4.789	2.240	0.05575	9.488	584	129300
anthracene	120127	178.12	45	4.534	4.457	2.240	0.1163	20.73	594	1300
phenanthrene	85018	178.23	1100	4.571	4.494	2.240	0.1073	19.13	596	34300
C1-fluorenes	-	180.25	??	4.720	4.640	2.240	0.07760	13.99	611	-
1-methylfluorene	1730376	180.25	1090	4.739	4.659	2.240	0.07445	13.42	612	49700
C4-naphthalenes	-	184.28	??	5.300	5.210	2.240	0.02197	4.048	657	-
2-methylanthracene	613127	192.26	29.99	4.991	4.906	2.240	0.04303	8.273	667	2420
1-methylanthracene	610480	192.26	??	4.998	4.913	2.240	0.04238	8.148	667	-
9-methylanthracene	779022	192.26	261.1	5.006	4.921	2.240	0.04165	8.007	668	21775
2-methylphenanthrene	2531842	192.26	??	5.029	4.944	2.240	0.03961	7.616	669	-
1-methylphenanthrene	832699	192.26	269.9	5.037	4.952	2.240	0.03893	7.485	670	24100
C1-phenanthrene/anthracenes	-	192.26	??	5.040	4.955	2.240	0.03868	7.436	670	-
9-ethylfluorene	2294828	194.28	??	4.973	4.889	2.240	0.04475	8.693	673	-
C2-fluorenes	-	194.27	??	5.200	5.112	2.240	0.02731	5.305	686	-
pyrene	129000	202.26	131.9	4.922	4.839	2.240	0.05000	10.11	697	9090
fluoranthene	206440	202.26	239.9	5.084	4.998	2.240	0.03515	7.109	707	23870
2-ethylanthracene	52251715	206.29	??	5.357	5.266	2.240	0.01940	4.003	739	-
C2-phenanthrene/anthracenes	-	206.29	??	5.460	5.367	2.240	0.01551	3.199	746	-
9,10-dimethylanthracene	781431	206.29	55.9	5.494	5.401	2.240	0.01440	2.971	748	14071
3,6-dimethylphenanthrene	1576676	206.29	??	5.515	5.422	2.240	0.01376	2.838	749	-
C3-fluorenes	-	208.30	??	5.700	5.603	2.240	0.009199	1.916	769	-
C1-pyrene/fluoranthenes	-	216.29	??	5.287	5.197	2.240	0.02260	4.887	770	-
2,3-benzofluorene	243174	216.28	2.001	5.539	5.445	2.240	0.01306	2.824	787	558
benzo(a)fluorene	238843	216.29	45.00	5.539	5.445	2.240	0.01306	2.824	787	12500
C3-phenanthrene/anthracenes	-	220.32	??	5.920	5.820	2.240	0.005700	1.256	829	-

Table 3-3. Results of approximate randomization (AR) test for the equality of the freshwater and saltwater FAV distributions at a K_{ow} of 1.0 and AR test for the equality of benthic and combined benthic and water column FAVs for freshwater and saltwater distributions.

Comparison	Habitat or Water Type ^a		AR Statistic ^b	Probability ^c
Fresh vs Salt	Fresh (20)	Salt (29)	5.746	93.5
Freshwater: Benthic vs WQC ^d	WQC (49)	Benthic (33)	0.862	82.8

^aValues in parantheses are the number of GMAVS at a K_{ow} of 1.0 used in the comparison.

^bAR statistic = FAV difference between original compared groups.

^cProbability that the theoretical AR statistic \leq the observed AR statistic given that all samples came from the same population.

^dCombined Freshwater and Saltwater.

Table 3-4. $C_{OC,PAH,FCV}$ concentrations at a K_{OW} of 1.0 and properties required for their derivation^A.

PAH ^B	CAS # ^C	Molecular Weight ($\mu\text{g}/\mu\text{mol}$)	Mackay Solid Solubility ^D ($\mu\text{g}/\text{L}$)	SPARC ^E $\log_{10}K_{OW}$	$\log_{10}K_{OC}$	FCV ($\mu\text{mol}/\text{g octanol}$)	PAH specific FCV ($\mu\text{mol}/\text{L}$)	PAH specific FCV ($\mu\text{g}/\text{L}$)	$C_{OC,PAH,FCV}$ ($\mu\text{g}/\text{goc}$)	$C_{OC,PAH,Max}^F$ ($\mu\text{g}/\text{goc}$)
indan	496117	118.18	100000	3.158	3.105	2.240	2.322	274.5	349	127200
naphthalene	91203	128.17	30995	3.356	3.299	2.240	1.509	193.5	385	61700
C1-naphthalenes	-	142.20	??	3.800	3.736	2.240	0.5744	81.69	444	-
1-methylnaphthalene	90120	142.20	28001	3.837	3.772	2.240	0.5300	75.37	446	165700
2-methylnaphthalene	91576	142.20	25000	3.857	3.792	2.240	0.5074	72.16	447	154800
acenaphthylene	208968	152.2	16314	3.223	3.168	2.240	2.016	306.9	452	24000
acenaphthene	83329	154.21	3800	4.012	3.944	2.240	0.3622	55.85	491	33400
1-ethylnaphthalene	1127760	156.23	10100	4.221	4.150	2.240	0.2298	35.91	507	142500
2-ethylnaphthalene	939275	156.23	8001	4.283	4.210	2.240	0.2008	31.37	509	129900
C2-naphthalenes	-	156.23	??	4.300	4.227	2.240	0.1935	30.24	510	-
1,4-dimethylnaphthalene	571584	156.23	11400	4.300	4.227	2.240	0.1935	30.24	510	192300
1,3-dimethylnaphthalene	575417	156.23	8001	4.367	4.293	2.240	0.1673	26.13	513	157100
2,6-dimethylnaphthalene	581420	156.23	1700	4.373	4.299	2.240	0.1651	25.79	513	33800
2,3-dimethylnaphthalene	581408	156.23	2500	4.374	4.300	2.240	0.1647	25.74	513	49900
1,5-dimethylnaphthalene	571619	156.23	3100	4.378	4.304	2.240	0.1633	25.52	514	62400
fluorene	86737	166.22	1900	4.208	4.137	2.240	0.2364	39.30	538	26000
C3-naphthalenes	-	170.25	??	4.800	4.719	2.240	0.06520	11.10	581	-
2,3,5-trimethylnaphthalene	2245387	170.26	??	4.858	4.776	2.240	0.05747	9.785	584	-
1,4,5-trimethylnaphthalene	213411	170.2	2100	4.872	4.789	2.240	0.05575	9.488	584	129300
anthracene	120127	178.12	45	4.534	4.457	2.240	0.1163	20.73	594	1300
phenanthrene	85018	178.23	1100	4.571	4.494	2.240	0.1073	19.13	596	34300
C1-fluorenes	-	180.25	??	4.720	4.640	2.240	0.07760	13.99	611	-
1-methylfluorene	1730376	180.25	1090	4.739	4.659	2.240	0.07445	13.42	612	49700
C4-naphthalenes	-	184.28	??	5.300	5.210	2.240	0.02197	4.048	657	-
2-methylanthracene	613127	192.26	29.99	4.991	4.906	2.240	0.04303	8.273	667	2420
1-methylanthracene	610480	192.26	??	4.998	4.913	2.240	0.04238	8.148	667	-
9-methylanthracene	779022	192.26	261.1	5.006	4.921	2.240	0.04165	8.007	668	21775
2-methylphenanthrene	2531842	192.26	??	5.029	4.944	2.240	0.03961	7.616	669	-
1-methylphenanthrene	832699	192.26	269.9	5.037	4.952	2.240	0.03893	7.485	670	24100
C1-phenanthrene/anthracenes	-	192.26	??	5.040	4.955	2.240	0.03868	7.436	670	-
9-ethylfluorene	2294828	194.28	??	4.973	4.889	2.240	0.04475	8.693	673	-
C2-fluorenes	-	194.27	??	5.200	5.112	2.240	0.02731	5.305	686	-
pyrene	129000	202.26	131.9	4.922	4.839	2.240	0.05000	10.11	697	9090
fluoranthene	206440	202.26	239.9	5.084	4.998	2.240	0.03515	7.109	707	23870
2-ethylanthracene	52251715	206.29	??	5.357	5.266	2.240	0.01940	4.003	739	-
C2-phenanthrene/anthracenes	-	206.29	??	5.460	5.367	2.240	0.01551	3.199	746	-
9,10-dimethylanthracene	781431	206.29	55.9	5.494	5.401	2.240	0.01440	2.971	748	14071
3,6-dimethylphenanthrene	1576676	206.29	??	5.515	5.422	2.240	0.01376	2.838	749	-
C3-fluorenes	-	208.30	??	5.700	5.603	2.240	0.009199	1.916	769	-
C1-pyrene/fluoranthenes	-	216.29	??	5.287	5.197	2.240	0.02260	4.887	770	-
2,3-benzofluorene	243174	216.28	2.001	5.539	5.445	2.240	0.01306	2.824	787	558
benzo(a)fluorene	238843	216.29	45.00	5.539	5.445	2.240	0.01306	2.824	787	12500
C3-phenanthrene/anthracenes	-	220.32	??	5.920	5.820	2.240	0.005700	1.256	829	-

PAH ^B	CAS # ^C	Molecular Weight ($\mu\text{g}/\mu\text{mol}$)	Mackay Solid Solubility ^D ($\mu\text{g}/\text{L}$)	SPARC ^E $\log_{10}K_{OW}$	$\log_{10}K_{OC}$	FCV ($\mu\text{mol}/\text{g octanol}$)	PAH specific FCV ($\mu\text{mol}/\text{L}$)	PAH specific FCV ($\mu\text{g}/\text{L}$)	$C_{OC,PAH,FCV}$ ($\mu\text{g}/\text{gOC}$)	$C_{OC,PAH,Max}$ ^F ($\mu\text{g}/\text{gOC}$)
naphthalene	92240	228.3	0.6000	5.633	5.538	2.240	0.01064	2.430	838	207
benz(a)anthracene	56553	228.29	11.00	5.673	5.577	2.240	0.009756	2.227	841	4153
chrysene	218019	228.29	2.000	5.713	5.616	2.240	0.008943	2.042	844	826
triphenylene	217594	228.3	43.00	5.752	5.654	2.240	0.008215	1.875	846	19400
C2-pyrene/fluoranthenes	-	230.13	??	5.800	5.702	2.240	0.007400	1.703	857	-
C4-phenanthrenes/anthracenes	-	234.23	??	6.320	6.213	2.240	0.002387	0.5594	913	-
C1-benzanthracene/chrysenes	-	242.32	??	6.140	6.036	2.240	0.003531	0.8557	929	-
C3-pyrene/fluoranthenes	-	244.32	??	6.284	6.177	2.240	0.002581	0.6307	949	-
benzo(a)pyrene	50328	252.31	3.810	6.107	6.003	2.240	0.003794	0.9573	965	3840
perylene	198550	252.31	0.4012	6.135	6.031	2.240	0.003570	0.9008	967	431
benzo(e)pyrene	192972	252.32	4.012	6.135	6.031	2.240	0.003570	0.9008	967	4300
benzo(b)fluoranthene	205992	252.32	1.501	6.266	6.160	2.240	0.002685	0.6774	979	2169
benzo(j)fluoranthene	205822	252.32	2.500	6.291	6.184	2.240	0.002542	0.6415	981	3820
benzo(k)fluoranthene	207089	252.32	0.7999	6.291	6.184	2.240	0.002542	0.6415	981	1220
C2-benzanthracene/chrysenes	-	256.23	??	6.429	6.320	2.240	0.001883	0.4827	1008	-
9,10-dimethylbenz(a)anthracene	56564	256.35	43.5	6.567	6.456	2.240	0.001395	0.3575	1021	124200
7,12-dimethylbenz(a)anthracene	57976	256.35	49.99	6.575	6.464	2.240	0.001370	0.3513	1021	145300
7-methylbenzo(a)pyrene	63041770	266.35	??	6.537	6.426	2.240	0.001489	0.3965	1058	-
benzo(ghi)perylene	191242	276.23	0.2600	6.507	6.397	2.240	0.001589	0.4391	1095	648
C3-benzanthracene/chrysenes	-	270.36	??	6.940	6.822	2.240	0.0006194	0.1675	1112	-
indeno(1,2,3-cd)pyrene	193395	276.23	??	6.722	6.608	2.240	0.0009953	0.2750	1115	-
dibenz(a,h)anthracene	53703	278.35	0.6012	6.713	6.599	2.240	0.001015	0.2825	1123	2389
dibenz(a,j)anthracene	58703	278.35	12.00	6.713	6.599	2.240	0.001015	0.2825	1123	47680
dibenz(a,c)anthracene	215587	278.35	1.601	6.780	6.665	2.240	0.0008773	0.2442	1129	7400
C4-benzanthracene/chrysenes	-	284.38	??	7.360	7.235	2.240	0.0002483	0.07062	1214	-
C1-dibenz(a,h)anthracenes	-	292.37	??	7.113	6.992	2.240	0.0004251	0.1243	1221	-
coronene	191071	300.36	0.1400	6.885	6.768	2.240	0.0006981	0.2097	1230	821
C2-dibenz(a,h)anthracenes	-	306.39	??	7.513	7.386	2.240	0.0001780	0.05454	1325	-
C3-dibenz(a,h)anthracenes	-	320.41	??	7.913	7.779	2.240	0.00007455	0.02389	1435	-

^AFour significant figures are used even when fewer are appropriate for the parameter to limit the effects of rounding error when calculating ΣESGTU_{FCV} which has two significant figures.

^BPAHs in bold are the 34 that constitute the minimum required to constitute "total PAH" for use in this PAH mixture ESG without correction for unmeasured PAHs.

^CFor C#-PAHs, a CAS is not available.

^DMackay et al., 1992. Illustrated handbook of physical chemical properties and Environmental Fate for organic chemicals. Volume 2.

^EFor C#-PAHs, reported $\log_{10}K_{OW}$ values are the average $\log_{10}K_{OW}$ values of several possible structural isomers.

^F $C_{OC,PAH,FCV}$ based on solubility; if $C_{OC,PAH,FCV}$ is $> C_{OC,PAH,Max}$, then this value replaces $C_{OC,PAH,FCV}$ in all calculations.

??Solubility is unknown

Table 4-1. ESGs for PAH mixtures: Example calculations for three sediments.

PAH ^a	$C_{OC, PAH, FCVI}$ ($\mu\text{g/g}_{OC}$) ^b	$C_{OC, PAH, Maxi}$ ($\mu\text{g/g}_{OC}$)	Sediment A (TOC=0.81%; f_{OC} =0.0081)			Sediment B (TOC=0.886%; f_{OC} =0.00886)			Sediment C (TOC=6.384%; f_{OC} =0.06384)		
			Conc. ($\mu\text{g/g dry wt.}$)	C_{OC} ($\mu\text{g/g}_{OC}$)	ESGTU _{FCVI}	Conc. ($\mu\text{g/g dry wt.}$)	C_{OC} ($\mu\text{g/g}_{OC}$)	ESGTU _{FCVI}	Conc. ($\mu\text{g/g dry wt.}$)	C_{OC} ($\mu\text{g/g}_{OC}$)	ESGTU _{FCVI}
acenaphthene	491	33400	0.000	0.00	0.00000	0.0401	4.53	0.00922	0.806	12.6	0.0257
acenaphthylene	452	24000	0.0348	4.29	0.00950	0.0165	1.86	0.00412	2.040	32.0	0.0707
anthracene	594	1300	0.628	77.6	0.1306	0.0507	5.72	0.00962	3.695	57.9	0.0974
benz(a)anthracene	841	4153	0.0709	8.75	0.0104	0.2011	22.69	0.02698	8.293	129.9	0.1545
benzo(a)pyrene	965	3840	0.164	20.3	0.0210	0.1817	20.51	0.02125	10.97	171.8	0.1781
benzo(c)pyrene	967	4300				0.1673	18.89	0.01953	8.920	139.7	0.1445
benzo(b)fluoranthene	979	2169	0.139	17.2	0.0175	0.1708	19.28	0.01969	18.14	284.1	0.2902
benzo(k)fluoranthene	981	1220	0.139	17.2	0.0175	0.1962	22.15	0.02258	5.500	86.2	0.0878
benzo(g,h,i)perylene	1095	648				0.1504	16.97	0.02619	5.583	87.5	0.1350
chrysene	844	826	0.157	19.4	0.0235	0.2574	29.05	0.03518	9.197	144.1	0.1744
dibenzo(a,h)anthracene	1123	2389				0.0423	4.77	0.00425	2.499	39.1	0.0349
fluoranthene	707	23870	0.0806	9.96	0.0141	0.3244	36.62	0.05180	2.519	39.5	0.0558
fluorene	538	26000	0.0722	8.91	0.0166	0.3702	41.78	0.07766	1.387	21.7	0.0404
indeno(1,2,3-cd)pyrene	1115	-				0.1473	16.63	0.01491	10.80	169.2	0.1517
naphthalene	385	61700	0.0894	11.0	0.0287	0.2703	30.51	0.07925	2.193	34.4	0.0892
perylene	967	431				0.3511	39.63	0.09194	28.23	442.2	1.0259
phenanthrene	596	34300	0.139	17.1	0.0287	0.5679	64.09	0.1075	4.208	65.9	0.1106
pyrene	697	9090	0.171	21.1	0.0303	0.4080	46.05	0.06606	20.14	315.5	0.4526
Cl chrysenes	929	-				0.2987	33.72	0.03629	5.240	82.1	0.0884
Cl fluoranthenes	770	-				0.3824	43.16	0.05605	11.73	183.7	0.2386
Cl fluorenes	611	-				0.9362	105.67	0.17294	1.030	16.1	0.0264
Cl naphthalenes	444	-				1.2084	136.39	0.30719	1.37	21.9	0.0493

PAH ^a	CAS # ^c	Molecular Weight ($\mu\text{g}/\mu\text{mol}$)	Mackay Solid Solubility ^d ($\mu\text{g}/\text{L}$)	SPARC ^e $\log_{10}K_{OW}$	$\log_{10}K_{OC}$	FCV ($\mu\text{mol}/\text{g octanol}$)	PAH specific FCV ($\mu\text{mol}/\text{L}$)	PAH specific FCV ($\mu\text{g}/\text{L}$)	$C_{OC,PAH,FCV}$ ($\mu\text{g}/\text{goc}$)	$C_{OC,PAH,Mari}$ ^f ($\mu\text{g}/\text{goc}$)
naphthacene	92240	228.3	0.6000	5.633	5.538	2.240	0.01064	2.430	838	207
benz(a)anthracene	56553	228.29	11.00	5.673	5.577	2.240	0.009756	2.227	841	4153
chrysene	218019	228.29	2.000	5.713	5.616	2.240	0.008943	2.042	844	826
triphenylene	217594	228.3	43.00	5.752	5.654	2.240	0.008215	1.875	846	19400
C2-pyrene/fluoranthenes	-	230.13	??	5.800	5.702	2.240	0.007400	1.703	857	-
C4-phenanthrenes/anthracenes	-	234.23	??	6.320	6.213	2.240	0.002387	0.5594	913	-
C1-benzanthracene/chrysenes	-	242.32	??	6.140	6.036	2.240	0.003531	0.8557	929	-
C3-pyrene/fluoranthenes	-	244.32	??	6.284	6.177	2.240	0.002581	0.6307	949	-
benzo(a)pyrene	50328	252.31	3.810	6.107	6.003	2.240	0.003794	0.9573	965	3840
perylene	198550	252.31	0.4012	6.135	6.031	2.240	0.003570	0.9008	967	431
benzo(e)pyrene	192972	252.32	4.012	6.135	6.031	2.240	0.003570	0.9008	967	4300
benzo(b)fluoranthene	205992	252.32	1.501	6.266	6.160	2.240	0.002685	0.6774	979	2169
benzo(j)fluoranthene	205822	252.32	2.500	6.291	6.184	2.240	0.002542	0.6415	981	3820
benzo(k)fluoranthene	207089	252.32	0.7999	6.291	6.184	2.240	0.002542	0.6415	981	1220
C2-benzanthracene/chrysenes	-	256.23	??	6.429	6.320	2.240	0.001883	0.4827	1008	-
9,10-dimethylbenz(a)anthracene	56564	256.35	43.5	6.567	6.456	2.240	0.001395	0.3575	1021	124200
7,12-dimethylbenz(a)anthracene	57976	256.35	49.99	6.575	6.464	2.240	0.001370	0.3513	1021	145300
7-methylbenzo(a)pyrene	63041770	266.35	??	6.537	6.426	2.240	0.001489	0.3965	1058	-
benzo(ghi)perylene	191242	276.23	0.2600	6.507	6.397	2.240	0.001589	0.4391	1095	648
C3-benzanthracene/chrysenes	-	270.36	??	6.940	6.822	2.240	0.0006194	0.1675	1112	-
indeno(1,2,3-cd)pyrene	193395	276.23	??	6.722	6.608	2.240	0.0009953	0.2750	1115	-
dibenz(a,h)anthracene	53703	278.35	0.6012	6.713	6.599	2.240	0.001015	0.2825	1123	2389
dibenz(a,j)anthracene	58703	278.35	12.00	6.713	6.599	2.240	0.001015	0.2825	1123	47680
dibenz(a,c)anthracene	215587	278.35	1.601	6.780	6.665	2.240	0.0008773	0.2442	1129	7400
C4-benzanthracene/chrysenes	-	284.38	??	7.360	7.235	2.240	0.0002483	0.07062	1214	-
C1-dibenz(a,h)anthracenes	-	292.37	??	7.113	6.992	2.240	0.0004251	0.1243	1221	-
coronene	191071	300.36	0.1400	6.885	6.768	2.240	0.0006981	0.2097	1230	821
C2-dibenz(a,h)anthracenes	-	306.39	??	7.513	7.386	2.240	0.0001780	0.05454	1325	-
C3-dibenz(a,h)anthracenes	-	320.41	??	7.913	7.779	2.240	0.00007455	0.02389	1435	-

^aFour significant figures are used even when fewer are appropriate for the parameter to limit the effects of rounding error when calculating ΣESGTU_{FCV} which has two significant figures.

^bPAHs in bold are the 34 that constitute the minimum required to constitute "total PAH" for use in this PAH mixture ESG without correction for unmeasured PAHs.

^cFor C#-PAHs, a CAS is not available.

^dMackay et al., 1992. Illustrated handbook of physical chemical properties and Environmental Fate for organic chemicals. Volume 2.

^eFor C#-PAHs, reported $\log_{10}K_{OW}$ values are the average $\log_{10}K_{OW}$ values of several possible structural isomers.

^f $C_{OC,PAH,FCV}$ based on solubility; if $C_{OC,PAH,FCV}$ is $> C_{OC,PAH,Mari}$, then this value replaces $C_{OC,PAH,FCV}$ in all calculations.

??Solubility is unknown

Table 4-1. ESGs for PAH mixtures: Example calculations for three sediments.

PAH ^a	$C_{OC, PAH, FCVI}$ ($\mu\text{g/g}_{OC}$) ^b	$C_{OC, PAH, Max}$ ($\mu\text{g/g}_{OC}$)	Sediment A (TOC=0.81%; f_{OC} =0.0081)			Sediment B (TOC=0.886%; f_{OC} =0.00886)			Sediment C (TOC=6.384%; f_{OC} =0.06384)		
			Conc. ($\mu\text{g/g dry wt.}$)	C_{OC} ($\mu\text{g/g}_{OC}$)	ESGTU _{FCVI}	Conc. ($\mu\text{g/g dry wt.}$)	C_{OC} ($\mu\text{g/g}_{OC}$)	ESGTU _{FCVI}	Conc. ($\mu\text{g/g dry wt.}$)	C_{OC} ($\mu\text{g/g}_{OC}$)	ESGTU _{FCVI}
acenaphthene	491	33400	0.000	0.00	0.00000	0.0401	4.53	0.00922	0.806	12.6	0.0257
acenaphthylene	452	24000	0.0348	4.29	0.00950	0.0165	1.86	0.00412	2.040	32.0	0.0707
anthracene	594	1300	0.628	77.6	0.1306	0.0507	5.72	0.00962	3.695	57.9	0.0974
benz(a)anthracene	841	4153	0.0709	8.75	0.0104	0.2011	22.69	0.02698	8.293	129.9	0.1545
benzo(a)pyrene	965	3840	0.164	20.3	0.0210	0.1817	20.51	0.02125	10.97	171.8	0.1781
benzo(e)pyrene	967	4300				0.1673	18.89	0.01953	8.920	139.7	0.1445
benzo(b)fluoranthene	979	2169	0.139	17.2	0.0175	0.1708	19.28	0.01969	18.14	284.1	0.2902
benzo(k)fluoranthene	981	1220	0.139	17.2	0.0175	0.1962	22.15	0.02258	5.500	86.2	0.0878
benzo(g,h,i)perylene	1095	648				0.1504	16.97	0.02619	5.583	87.5	0.1350
chrysene	844	826	0.157	19.4	0.0235	0.2574	29.05	0.03518	9.197	144.1	0.1744
dibenzo(a,h)anthracene	1123	2389				0.0423	4.77	0.00425	2.499	39.1	0.0349
fluoranthene	707	23870	0.0806	9.96	0.0141	0.3244	36.62	0.05180	2.519	39.5	0.0558
fluorene	538	26000	0.0722	8.91	0.0166	0.3702	41.78	0.07766	1.387	21.7	0.0404
indeno(1,2,3-cd)pyrene	1115	-				0.1473	16.63	0.01491	10.80	169.2	0.1517
naphthalene	385	61700	0.0894	11.0	0.0287	0.2703	30.51	0.07925	2.193	34.4	0.0892
perylene	967	431				0.3511	39.63	0.09194	28.23	442.2	1.0259
phenanthrene	596	34300	0.139	17.1	0.0287	0.5679	64.09	0.1075	4.208	65.9	0.1106
pyrene	697	9090	0.171	21.1	0.0303	0.4080	46.05	0.06606	20.14	315.5	0.4526
C1 chrysenes	929	-				0.2987	33.72	0.03629	5.240	82.1	0.0884
C1 fluoranthenes	770	-				0.3824	43.16	0.05605	11.73	183.7	0.2386
C1 fluorenes	611	-				0.9362	105.67	0.17294	1.030	16.1	0.0264
C1 naphthalenes	444	-				1.2084	136.39	0.30719	1.37	21.9	0.0493

C1 phenanthrenes	670	-	0.9267	104.6	0.15611	4.559	71.4	0.1066
C2 chrysenes	1008	-	0.2242	25.30	0.02510	4.753	74.5	0.0739
C2 flourenes	686	-	1.2384	139.77	0.20375	1.928	30.2	0.0440
C2 naphthalenes	510	-	3.2691	368.98	0.72348	1.448	22.7	0.0445
C2 phenanthrenes	746	-	1.0645	120.15	0.16106	4.789	75.0	0.1006
C3 chrysenes	1112	-	0.0279	3.15	0.00283	0.398	6.2	0.0056
C3 flourenes	769	-	1.2664	142.94	0.18587	3.419	53.6	0.0696
C3 naphthalenes	581	-	5.1079	576.51	0.99227	1.979	31.0	0.0533
C3 phenanthrenes	829	-	0.8100	91.43	0.11028	5.378	84.2	0.1016
C4 chrysenes	1214	-	0.1196	13.5	0.01112	1.581	24.8	0.0204
C4 naphthalenes	657	-	3.3088	373.46	0.56843	2.009	31.5	0.0479
C4 phenanthrenes	913	-	0.5644	63.71	0.06978	4.674	73.2	0.0802
Sum total of ESGTU _{FCVI}			$\Sigma \text{ESGTU}_{\text{FCVI}} = 0.348$		$\Sigma \text{ESGTU}_{\text{FCVI,TOT}} = 4.470$		$\Sigma \text{ESGTU}_{\text{FCVI,TOT}} = 4.470$	

a PAHs and corresponding $C_{\text{OC,PAH,FCVI}}$ and $C_{\text{OC,PAH,Max}}$ values are from Table 3-4 (bold).

b $C_{\text{OC,PAH,FCVI}}$ based on solubility, if $C_{\text{OC,PAH,FCVI}}$ exceeds the $C_{\text{OC,PAH,Max}}$ (i.e., benzo(g,h,i)perylene, chrysene, and perylene) then $C_{\text{OC,PAH,Max}}$ is used to calculate ESGTU_{FCVI}

Table 5-1. Water-only and spiked-sediment LC50 values used to test the applicability of narcosis and equilibrium partitioning theories to the derivation of ESGs for PAHs.

Test Species	Chemical	Method ^A	Water-only LC50 (µg/L)	Interstitial Water LC50 (µg/L)	Ratio: Interstitial Water LC50/Water-only LC50	Organic Carbon-Normalized LC50 (µg/g _{OC})			Reference
						Observed	Predicted ^B	LC50 Ratio Obs/Pred	
<u>Freshwater</u>									
<i>Diporeia</i> sp.	Fluoranthene	FT,M/10	>194	>381.3	-	-	-	-	Landrum, 1995
<i>Hyalella azteca</i>	Fluoranthene	FT,M/10	130.7	>75.4	> 0.58	-	-	-	Landrum, 1995
<i>Hyalella azteca</i>	Fluoranthene	S,M/10	44.9	45.9	1.02 ^C	500	4490	0.11 ^C	Suedel et al., 1993
<i>Hyalella azteca</i>	Fluoranthene	S,M/10	44.9	236.5	5.27 ^C	1480	4490	0.33 ^C	Suedel et al., 1993
<i>Hyalella azteca</i>	Fluoranthene	S,M/10	44.9	97.6	2.17 ^C	1250	4490	0.28 ^C	Suedel et al., 1993
<i>Chironomus tentans</i>	Fluoranthene	S,M/10	31.9	91.2	2.86 ^C	1587	3190	0.50 ^C	Suedel et al., 1993
<i>Chironomus tentans</i>	Fluoranthene	S,M/10	31.9	251	7.87 ^C	1740	3190	0.55 ^C	Suedel et al., 1993
<i>Chironomus tentans</i>	Fluoranthene	S,M/10	31.9	75.7	2.37 ^C	682	3190	0.21 ^C	Suedel et al., 1993
<u>Saltwater</u>									
<i>Eohaustorius estuarius</i>	Acenaphthene	FT,M/10	374	800	2.14	4330	2152	2.01	Swartz, 1991a
<i>Eohaustorius estuarius</i>	Acenaphthene	FT,M/10	374	609	1.63	1920	2152	0.89	Swartz, 1991a
<i>Eohaustorius estuarius</i>	Acenaphthene	FT,M/10	374	542	1.45	1630	2152	0.76	Swartz, 1991a
<i>Leptocheirus plumulosus</i>	Acenaphthene	FT,M/10	678	> 1,720	> 2.54	> 23,500	3900	> 6.02	Swartz, 1991a
<i>Leptocheirus plumulosus</i>	Acenaphthene	FT,M/10	678	1410	2.08	7730	3900	1.98	Swartz, 1991a
<i>Leptocheirus plumulosus</i>	Acenaphthene	FT,M/10	678	1490	2.20	11200	3900	2.87	Swartz, 1991a
<i>Eohaustorius estuarius</i>	Phenanthrene	FT,M/10	131	138	1.05	4050	3778	1.07	Swartz, 1991a
<i>Eohaustorius estuarius</i>	Phenanthrene	FT,M/10	131	139	1.06	3920	3778	1.04	Swartz, 1991a
<i>Eohaustorius estuarius</i>	Phenanthrene	FT,M/10	131	146	1.11	3820	3778	1.01	Swartz, 1991a
<i>Leptocheirus plumulosus</i>	Phenanthrene	FT,M/10	185	387	2.09	8200	5335	1.54	Swartz, 1991a
<i>Leptocheirus plumulosus</i>	Phenanthrene	FT,M/10	185	306	1.65	6490	5335	1.22	Swartz, 1991a
<i>Leptocheirus plumulosus</i>	Phenanthrene	FT,M/10	185	360	1.95	8200	5335	1.54	Swartz, 1991a
<i>Rhepoxynius abronius</i>	2,6-dimethylnaphthlene	S,M/10	-	200	-	8120	-	-	Ozretich et al., 2000a
<i>Rhepoxynius abronius</i>	2,3,5-trimethylnaphthlene	S,M/10	-	153	-	3190	-	-	Ozretich et al., 2000a
<i>Rhepoxynius abronius</i>	1-methylfluorene	S,M/10	-	44	-	1950	-	-	Ozretich et al., 2000a
<i>Rhepoxynius abronius</i>	2-methylphenanthrene	S,M/10	-	70	-	2270	-	-	Ozretich et al., 2000a
<i>Rhepoxynius abronius</i>	9-methylanthracene	S,M/10	-	32	-	6840	-	-	Ozretich et al., 2000a
<i>Rhepoxynius abronius</i>	Acenaphthene	S,M/10	-	-	-	2110	-	-	Swartz et al., 1997
<i>Rhepoxynius abronius</i>	Acenaphthene	S,M/10	-	-	-	2310	-	-	Swartz et al., 1997
<i>Rhepoxynius abronius</i>	Naphthalene	S,M/10	-	10440	-	31000	-	-	Ozretich et al., 2000a
<i>Rhepoxynius abronius</i>	Phenanthrene	S,M/10	-	-	-	3080	-	-	Swartz et al., 1997
<i>Rhepoxynius abronius</i>	Phenanthrene	S,M/10	-	-	-	2220	-	-	Swartz et al., 1997
<i>Rhepoxynius abronius</i>	Pyrene	S,M/10	-	28.1	-	1610	-	-	Ozretich et al., 2000a
<i>Rhepoxynius abronius</i>	Pyrene	S,M/10	-	-	-	1220	-	-	Swartz et al., 1997
<i>Rhepoxynius abronius</i>	Pyrene	S,M/10	-	-	-	2810	-	-	Swartz et al., 1997
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	-	-	2320	1390	1.66	Swartz et al., 1997
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	-	-	3310	1390	2.38	Swartz et al., 1997

C1 phenanthrenes	670	-	0.9267	104.6	0.15611	4.559	71.4	0.1066
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						Observed	Predicted ^B	LC50 Ratio Obs/Pred	
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<i>Hyaella azteca</i>	Fluoranthene	FT,M/10	130.7	>75.4	> 0.58	-	-	-	Landrum, 1995
<i>Hyaella azteca</i>	Fluoranthene	S,M/10	44.9	45.9	1.02 ^C	500	4490	0.11 ^C	Suedel et al., 1993
<i>Hyaella azteca</i>	Fluoranthene	S,M/10	44.9	236.5	5.27 ^C	1480	4490	0.33 ^C	Suedel et al., 1993
<i>Hyaella azteca</i>	Fluoranthene	S,M/10	44.9	97.6	2.17 ^C	1250	4490	0.28 ^C	Suedel et al., 1993
<i>Chironomus tentans</i>	Fluoranthene	S,M/10	31.9	91.2	2.86 ^C	1587	3190	0.50 ^C	Suedel et al., 1993
<i>Chironomus tentans</i>	Fluoranthene	S,M/10	31.9	251	7.87 ^C	1740	3190	0.55 ^C	Suedel et al., 1993
<i>Chironomus tentans</i>	Fluoranthene	S,M/10	31.9	75.7	2.37 ^C	682	3190	0.21 ^C	Suedel et al., 1993
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<i>Eohaustorius estuarius</i>	Acenaphthene	FT,M/10	374	542	1.45	1630	2152	0.76	Swartz, 1991a
<i>Leptocheirus plumulosus</i>	Acenaphthene	FT,M/10	678	>1,720	> 2.54	>23,500	3900	> 6.02	Swartz, 1991a
<i>Leptocheirus plumulosus</i>	Acenaphthene	FT,M/10	678	1410	2.08	7730	3900	1.98	Swartz, 1991a
<i>Leptocheirus plumulosus</i>	Acenaphthene	FT,M/10	678	1490	2.20	11200	3900	2.87	Swartz, 1991a
<i>Eohaustorius estuarius</i>	Phenanthrene	FT,M/10	131	138	1.05	4050	3778	1.07	Swartz, 1991a
<i>Eohaustorius estuarius</i>	Phenanthrene	FT,M/10	131	139	1.06	3920	3778	1.04	Swartz, 1991a
<i>Eohaustorius estuarius</i>	Phenanthrene	FT,M/10	131	146	1.11	3820	3778	1.01	Swartz, 1991a
<i>Leptocheirus plumulosus</i>	Phenanthrene	FT,M/10	185	387	2.09	8200	5335	1.54	Swartz, 1991a
<i>Leptocheirus plumulosus</i>	Phenanthrene	FT,M/10	185	306	1.65	6490	5335	1.22	Swartz, 1991a
<i>Leptocheirus plumulosus</i>	Phenanthrene	FT,M/10	185	360	1.95	8200	5335	1.54	Swartz, 1991a
<i>Rhepoxynius abronius</i>	2,6-dimethylnaphthlene	S,M/10	-	200	-	8120	-	-	Ozretich et al., 2000a
<i>Rhepoxynius abronius</i>	2,3,5-trimethylnaphthlene	S,M/10	-	153	-	3190	-	-	Ozretich et al., 2000a
<i>Rhepoxynius abronius</i>	1-methylfluorene	S,M/10	-	44	-	1950	-	-	Ozretich et al., 2000a
<i>Rhepoxynius abronius</i>	2-methylphenanthrene	S,M/10	-	70	-	2270	-	-	Ozretich et al., 2000a
<i>Rhepoxynius abronius</i>	9-methylanthracene	S,M/10	-	32	-	6840	-	-	Ozretich et al., 2000a
<i>Rhepoxynius abronius</i>	Acenaphthene	S,M/10	-	-	-	2110	-	-	Swartz et al., 1997
<i>Rhepoxynius abronius</i>	Acenaphthene	S,M/10	-	-	-	2310	-	-	Swartz et al., 1997
<i>Rhepoxynius abronius</i>	Naphthalene	S,M/10	-	10440	-	31000	-	-	Ozretich et al., 2000a
<i>Rhepoxynius abronius</i>	Phenanthrene	S,M/10	-	-	-	3080	-	-	Swartz et al., 1997
<i>Rhepoxynius abronius</i>	Phenanthrene	S,M/10	-	-	-	2220	-	-	Swartz et al., 1997
<i>Rhepoxynius abronius</i>	Pyrene	S,M/10	-	28.1	-	1610	-	-	Ozretich et al., 2000a
<i>Rhepoxynius abronius</i>	Pyrene	S,M/10	-	-	-	1220	-	-	Swartz et al., 1997
<i>Rhepoxynius abronius</i>	Pyrene	S,M/10	-	-	-	2810	-	-	Swartz et al., 1997
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	-	-	2320	1390	1.66	Swartz et al., 1997
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	-	-	3310	1390	2.38	Swartz et al., 1997

<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	22.7	1.63	1890	1390	1.36	Swartz et al., 1990
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	29.4	2.12	2100	1390	1.51	Swartz et al., 1990
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	24.2	1.74	2230	1390	1.60	Swartz et al., 1990
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	> 315	> 22.66 ^D	> 4360	1390	4.04 ^D	DeWitt et al., 1992
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	14.1	1.01	4410	1390	3.17	DeWitt et al., 1992
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	26.6	1.91	3080	1390	2.22	DeWitt et al., 1992
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	19.2	1.38	3150	1390	2.26	DeWitt et al., 1992
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	9.38	0.67	2790	1390	2.01	DeWitt et al., 1992
				Mean LC50 ratio =		1.60	Mean LC50 ratio =		1.91

^aTest conditions for water-only toxicity tests: S = static, FT = flow-through, M = measured, 10 = 10-d duration.

^bPredicted LC50 ($\mu\text{g/g}_{\text{OC}}$) = water-only LC50 ($\mu\text{g/L}$) \times K_{OC} (L/kg_{OC}) \times 1 kg_{OC}/1000g_{OC}.

^cSediments spiked with fluoranthene by Suedel et al. (1993) were not at equilibrium, therefore, are not included in the mean.

^dSource of organic carbon was fresh plant material, not naturally aged organic matter, therefore, value was not included in the mean.

^e10-day LC50 value from Swartz (2000).

Table 5-2. Percent mortality of benthic invertebrates in relation to the Σ ESGTU_{FCV} values of mixtures of polycyclic aromatic hydrocarbons spiked into sediment.

Species ^A	Σ ESGTU _{FCV} PAH Kow < 5.5	Σ ESGTU _{FCV} PAH Kow > 5.5	Σ ESGTU _{FCV} All PAHs	Percent Mortality	PAH Mixture ^B	Reference
<i>Diporeia sp.</i>	0.01	0.02	0.03	3	fluor, phen, anthr, flu, pyr, chry, b(b)flu, b(e)pyr, b(a)pyr, pery, b(ghi)pery	Landrum et al., 1991
<i>Diporeia sp.</i>	0.21	0.36	0.57	10	fluor, phen, anthr, flu, pyr, chry, b(b)flu, b(e)pyr, b(a)pyr, pery, b(ghi)pery	Landrum et al., 1991
<i>Diporeia sp.</i>	0.49	0.60	1.10	0	fluor, phen, anthr, flu, pyr, chry, b(b)flu, b(e)pyr, b(a)pyr, pery, b(ghi)pery	Landrum et al., 1991
<i>Diporeia sp.</i>	1.37	1.71	3.08	12	fluor, phen, anthr, flu, pyr, chry, b(b)flu, b(e)pyr, b(a)pyr, pery, b(ghi)pery	Landrum et al., 1991
<i>R. abronius</i>	10.32	0	10.3	100	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	5.80	0	5.80	38	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	5.12	0	5.12	8	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	3.25	0	3.25	11	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	2.50	0	2.50	4	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	1.80	0	1.80	2	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	1.42	0	1.42	3	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	2.77	0	2.77	5	anthr; flu	Boese et al., 1999
<i>R. abronius</i>	4.91	5.02	9.93	3	b(a)anthr; flu	Boese et al., 1999
<i>R. abronius</i>	5.88	0	5.88	5	2-methylanthr; flu	Boese et al., 1999
<i>R. abronius</i>	5.71	0	5.71	2	9,10-dimethylanthr; flu	Boese et al., 1999
<i>R. abronius</i>	2.71	2.23	4.94	3	b(b)flu; flu	Boese et al., 1999
<i>R. abronius</i>	2.06	0.79	2.84	2	chr; flu	Boese et al., 1999
<i>R. abronius</i>	0.63	1.57	2.20	1	3,6-dimethylphen; flu	Boese et al., 1999
<i>R. abronius</i>	1.91	25.89	27.8	4	anthr; b(a)anthr; 2-methylanthr; b(b)flu; chr; 3,6-dimethylphen	Boese et al., 1999
<i>R. abronius</i>	0.58	8.03	8.61	5	anthr; b(a)anthr; 2-methylanthr; b(b)flu; chr; 3,6-dimethylphen	Boese et al., 1999
<i>R. abronius</i>	1.55	8.03	9.58	9	anthr; b(a)anthr; 2-methylanthr; b(b)flu; chry; 3,6-dimethylphen; flu	Boese et al., 1999
<i>R. abronius</i>	0.90	3.40	4.30	0	anthr; b(a)anthr; 2-methylanthr; b(b)flu; chry; 3,6-dimethylphen; flu	Boese et al., 1999
<i>A. abdita</i>	5.41	0.64	6.05	7	9,10-dimethylanthr; chry	Burgess et al., 2000
<i>A. abdita</i>	0	2.58	2.58	7	b(a)pyr; cor	Burgess et al., 2000
<i>A. abdita</i>	5.41	3.22	8.63	10	9,10-dimethylanthr; chry; b(a)pyr; cor	Burgess et al., 2000
<i>A. bahia</i>	5.41	0.64	6.05	3	9,10-dimethylanthr; chry	Burgess et al., 2000
<i>A. bahia</i>	0	2.58	2.58	7	b(a)pyr; cor	Burgess et al., 2000
<i>A. bahia</i>	5.41	3.22	8.63	7	9,10-dimethylanthr; chry; b(a)pyr; cor	Burgess et al., 2000

^ATest Species: amphipods: *Diporeia sp.*, *Rhepoxynius abronius*, *Ampelisca abdita*; mysids: *Americamysis bahia*

^BPAH Code: ace - acenaphthene; anthr - anthracene; b(a)anthr - benz(a)anthracene; b(a)pyr - benzo(a)pyrene; b(ghi)pery - benzo(ghi)perylene; b(b)flu - benzo(b)fluoranthene; chry - chrysene; cor - coronene; 9,10-dimethylanthr - 9,10-dimethylanthrane; 3,6-dimethylphen - 3,6-dimethylphenanthrene; flu - fluoranthene; fluo - fluorene; 2-methylanthr - 2-methylanthrane; pery - perylene; phen - phenanthrene; pyr - pyrene.

<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	22.7	1.63	1890	1390	1.36	Swartz et al., 1990
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	29.4	2.12	2100	1390	1.51	Swartz et al., 1990
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	24.2	1.74	2230	1390	1.60	Swartz et al., 1990
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	> 315	> 22.66 ^D	> 4360	1390	4.04 ^D	DeWitt et al., 1992
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	14.1	1.01	4410	1390	3.17	DeWitt et al., 1992
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	26.6	1.91	3080	1390	2.22	DeWitt et al., 1992
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	19.2	1.38	3150	1390	2.26	DeWitt et al., 1992
<i>Rhepoxynius abronius</i>	Fluoranthene	S,M/10	13.9 ^E	9.38	0.67	2790	1390	2.01	DeWitt et al., 1992
Mean LC50 ratio =					1.60	Mean LC50 ratio =			1.91

^ETest conditions for water-only toxicity tests: S = static, FT = flow-through, M = measured, 10 = 10-d duration.

^DPredicted LC50 ($\mu\text{g}/\text{g}_{\text{OC}}$) = water-only LC50 ($\mu\text{g}/\text{L}$) \times K_{OC} ($\text{L}/\text{kg}_{\text{OC}}$) \times 1 $\text{kg}_{\text{OC}}/1000\text{g}_{\text{OC}}$.

^CSediments spiked with fluoranthene by Suedel et al. (1993) were not at equilibrium, therefore, are not included in the mean.

^FSource of organic carbon was fresh plant material, not naturally aged organic matter, therefore, value was not included in the mean.

¹⁰10-day LC50 value from Swartz (2000).

Table 5-2. Percent mortality of benthic invertebrates in relation to the Σ ESGTU_{FCV} values of mixtures of polycyclic aromatic hydrocarbons spiked into sediment.

Species ^a	Σ ESGTU _{FCV} PAH Kow <5.5	Σ ESGTU _{FCV} PAH Kow >5.5	Σ ESGTU _{FCV} All PAHs	Percent Mortality	PAH Mixture ^b	Reference
<i>Diporeia sp.</i>	0.01	0.02	0.03	3	fluor, phen, anthr, flu, pyr, chry, b(b)flu, b(e)pyr, b(a)pyr, pery, b(ghi)pery	Landrum et al., 1991
<i>Diporeia sp.</i>	0.21	0.36	0.57	10	fluor, phen, anthr, flu, pyr, chry, b(b)flu, b(e)pyr, b(a)pyr, pery, b(ghi)pery	Landrum et al., 1991
<i>Diporeia sp.</i>	0.49	0.60	1.10	0	fluor, phen, anthr, flu, pyr, chry, b(b)flu, b(e)pyr, b(a)pyr, pery, b(ghi)pery	Landrum et al., 1991
<i>Diporeia sp.</i>	1.37	1.71	3.08	12	fluor, phen, anthr, flu, pyr, chry, b(b)flu, b(e)pyr, b(a)pyr, pery, b(ghi)pery	Landrum et al., 1991
<i>R. abronius</i>	10.32	0	10.3	100	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	5.80	0	5.80	38	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	5.12	0	5.12	8	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	3.25	0	3.25	11	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	2.50	0	2.50	4	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	1.80	0	1.80	2	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	1.42	0	1.42	3	ace; phen; flu; pyr	Swartz et al., 1997
<i>R. abronius</i>	2.77	0	2.77	5	anthr; flu	Boese et al., 1999
<i>R. abronius</i>	4.91	5.02	9.93	3	b(a)anthr; flu	Boese et al., 1999
<i>R. abronius</i>	5.88	0	5.88	5	2-methylanthr; flu	Boese et al., 1999
<i>R. abronius</i>	5.71	0	5.71	2	9,10-dimethylanthr; flu	Boese et al., 1999
<i>R. abronius</i>	2.71	2.23	4.94	3	b(b)flu; flu	Boese et al., 1999
<i>R. abronius</i>	2.06	0.79	2.84	2	chr; flu	Boese et al., 1999
<i>R. abronius</i>	0.63	1.57	2.20	1	3,6-dimethylphen; flu	Boese et al., 1999
<i>R. abronius</i>	1.91	25.89	27.8	4	anthr; b(a)anthr; 2-methylanthr; b(b)flu; chr; 3,6-dimethylphen	Boese et al., 1999
<i>R. abronius</i>	0.58	8.03	8.61	5	anthr; b(a)anthr; 2-methylanthr; b(b)flu; chr; 3,6-dimethylphen	Boese et al., 1999
<i>R. abronius</i>	1.55	8.03	9.58	9	anthr; b(a)anthr; 2-methylanthr; b(b)flu; chry; 3,6-dimethylphen; flu	Boese et al., 1999
<i>R. abronius</i>	0.90	3.40	4.30	0	anthr; b(a)anthr; 2-methylanthr; b(b)flu; chry; 3,6-dimethylphen; flu	Boese et al., 1999
<i>A. abdita</i>	5.41	0.64	6.05	7	9,10-dimethylanthr; chry	Burgess et al., 2000
<i>A. abdita</i>	0	2.58	2.58	7	b(a)pyr; cor	Burgess et al., 2000
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<i>A. bahia</i>	0	2.58	2.58	7	b(a)pyr; cor	Burgess et al., 2000
<i>A. bahia</i>	5.41	3.22	8.63	7	9,10-dimethylanthr; chry; b(a)pyr; cor	Burgess et al., 2000

^aTest Species: amphipods: *Diporeia sp.*, *Rhepoxynius abronius*, *Ampelisca abdita*; mysids: *Americamysis bahia*

^bPAH Code: ace - acenaphthene; anthr - anthracene; b(a)anthr - benz(a)anthracene; b(a)pyr - benzo(a)pyrene; b(ghi)pery - benzo(ghi)perylene; b(b)flu - benzo(b)fluoranthene; chry - chrysene; cor - coronene; 9,10-dimethylanthr - 9,10-dimethylanthrane; 3,6-dimethylphen - 3,6-dimethylphenanthrene; flu - fluoranthene; fluor - fluorene; 2-methylanthr - 2-methylanthrane; pery - perylene; phen - phenanthrene; pyr - pyrene.

Table 5-3. Chemicals included in the high K_{ow} PAH mixture experiment (Spehar et al., 2000).

Chemical Name	Molecular Weight (g/mol)	$\log_{10} K_{ow}^a$	$\log_{10} K_{oc}^b$	Estimated Solubility ^c ($\mu\text{g/L}$)	Target Sediment Concentration ($\mu\text{mol/g}_{oc}$)	Nominal Water Concentration ^d ($\mu\text{g/L}$)	Solubility Limited Nominal Water Concentration ($\mu\text{g/L}$)
3,6-Dimethylphenanthrene	206.29	5.52	5.42	77.98	42.38	33.12	33.12
2-Ethylanthracene	206.29	5.36	5.27	59.62	39.32	43.94	43.94
2-(tert-butyl)anthracene	234.34	5.88	5.78	33.04	50.91	19.78	19.78
2,3 Benzofluorene	216.28	5.54	5.44	25.30	42.88	33.27	25.30
Benzo(a)anthracene	228.29	5.67	5.58	12.28	45.80	27.70	12.28
Triphenylene	228.30	5.75	5.65	5.110	47.66	24.11	5.110
9-Phenylanthracene	254.33	6.31	6.20	3.640	64.22	10.30	3.640
Benzo(b)fluoranthene	252.32	6.27	6.16	8.280	62.75	10.96	8.280
Benzo(k)fluoranthene	252.32	6.29	6.18	8.350	63.64	10.50	8.350
7,12-Dimethylbenz(a)anthracene	256.35	6.58	6.46	13.41	75.04	6.620	6.620
Benzo(a)pyrene	252.31	6.11	6.00	2.880	57.46	14.38	2.880
3-Methylcholanthrene	268.38	6.76	6.64	3.110	83.92	5.100	3.110
7-Methylbenzo(a)pyrene	266.35	6.54	6.43	1.460	73.37	7.320	1.460
TOTAL PAH- WATER CONCENTRATION					749.4	247.1	173.9

^aPredicted by SPARC in distilled water at 25°C.

^bPredicted from Di Toro et al. (1991).

^cNominal concentration predicted by K_{oc} , regardless of solubility limits; highest concentration only.

^dTarget sediment concentration/ K_{oc} .

Table 6-1. Relative Distribution of $\Sigma\text{ESGTU}_{\text{FCV,TOT}}$ to $\Sigma\text{ESGTU}_{\text{FCV,13}}$ and $\Sigma\text{ESGTU}_{\text{FCV,23}}$ for the Combined EMAP Dataset (N=488).

Percentile	$\Sigma\text{ESGTU}_{\text{FCV,TOT}} / \Sigma\text{ESGTU}_{\text{FCV,13}}$	$\Sigma\text{ESGTU}_{\text{FCV,TOT}} / \Sigma\text{ESGTU}_{\text{FCV,23}}$
50	2.75	1.64
80	6.78	2.80 ^a
90	8.45	3.37
95	11.5	4.14
99	16.9	6.57

Table 5-3. Chemicals included in the high K_{ow} PAH mixture experiment (Spehar et al., 2000).

Chemical Name	Molecular Weight (g/mol)	$\log_{10} K_{ow}^a$	$\log_{10} K_{oc}^b$	Estimated Solubility ^c ($\mu\text{g/L}$)	Target Sediment Concentration ($\mu\text{mol/g}_{oc}$)	Nominal Water Concentration ^d ($\mu\text{g/L}$)	Solubility Limited Nominal Water Concentration ($\mu\text{g/L}$)
3,6-Dimethylphenanthrene	206.29	5.52	5.42	77.98	42.38	33.12	33.12
2-Ethylanthracene	206.29	5.36	5.27	59.62	39.32	43.94	43.94
2-(tert-butyl)anthracene	234.34	5.88	5.78	33.04	50.91	19.78	19.78
2,3 Benzofluorene	216.28	5.54	5.44	25.30	42.88	33.27	25.30
Benzo(a)anthracene	228.29	5.67	5.58	12.28	45.80	27.70	12.28
Triphenylene	228.30	5.75	5.65	5.110	47.66	24.11	5.110
9-Phenylanthracene	254.33	6.31	6.20	3.640	64.22	10.30	3.640
Benzo(b)fluoranthene	252.32	6.27	6.16	8.280	62.75	10.96	8.280
Benzo(k)fluoranthene	252.32	6.29	6.18	8.350	63.64	10.50	8.350
7,12-Dimethylbenz(a)anthracene	256.35	6.58	6.46	13.41	75.04	6.620	6.620
Benzo(a)pyrene	252.31	6.11	6.00	2.880	57.46	14.38	2.880
3-Methylcholanthrene	268.38	6.76	6.64	3.110	83.92	5.100	3.110
7-Methylbenzo(a)pyrene	266.35	6.54	6.43	1.460	73.37	7.320	1.460
TOTAL PAH- WATER CONCENTRATION					749.4	247.1	173.9

^aPredicted by SPARC in distilled water at 25°C.

^bPredicted from Di Toro et al. (1991).

^cNominal concentration predicted by K_{oc} , regardless of solubility limits; highest concentration only.

^dTarget sediment concentration/ K_{oc} .

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Percentile	$\Sigma\text{ESGTU}_{\text{FCV,TOT}} / \Sigma\text{ESGTU}_{\text{FCV,13}}$	$\Sigma\text{ESGTU}_{\text{FCV,TOT}} / \Sigma\text{ESGTU}_{\text{FCV,23}}$
50	2.75	1.64
80	6.78	2.80
90	8.45	3.37
95	11.5	4.14
99	16.9	6.57

Table 6-2. PAH measured in various sediment monitoring programs. See Di Toro and McGrath (2000) for data sources.

Parameter	NOAA	SFEI	San Diego	Southern California	NY/NJ REMAP ^A	Virginian EMAP ^B	Elliott Bay	Carolinian EMAP	Louisian EMAP
Acenaphthene	x	x	x	x	x	x	x	x	x
Acenaphthylene	x	x	x	x	x	x	x	x	x
Anthracene	x	x	x	x	x	x	x	x	x
Chrysene	x	x	x	x	x	x	x	x	x
Fluoranthene	x	x	x	x	x	x	x	x	x
Fluorene	x	x	x	x	x	x	x	x	x
naphthalene	x	x	x	x	x	x	x	x	x
phenanthrene	x	x	x	x	x	x	x	x	x
pyrene	x	x	x	x	x	x	x	x	x
Benzo(k)fluoranthene	x	x	x	x	x	x	x	x	x
Benzo(b)fluoranthene	x	x	x	x	x	x	x	x	x
Benzo(a)pyrene	x	x	x	x	x	x	x	x	x
Benzo(a)anthracene	x	x	x	x	x	x	x	x	x
Benzo(e)pyrene	x	x	x	x	x	x	x	x	x
Benzo(g,h,i)perylene	x	x	x	x	x	x	x	x	x
Dibenz(a,h)anthracene	x	x	x	x	x	x	x	x	x
2,6-dimethylnaphthalene	x	x	x	x	x	x	x	x	x
Indeno(1,2,3-cd)pyrene	x	x	x	x	x	x	x	x	x
1-methylnaphthalene	x	x	x	x	x	x	x	x	x
2-methylnaphthalene	x	x	x	x	x	x	x	x	x
perylene	x	x	x	x	x	x	x	x	x
1-methylphenanthrene	x	x	x	x	x	x	x	x	x
2,3,5-trimethylnaphthalene	x	x	x	x	x	x	x	x	x
2-methylantracene							x		
2-methylphenanthrene		x					x		
3,6-dimethylphenanthrene							x		
9-methylantracene		x					x		
9,10-dimethylantracene							x		
C1-benzo(a)anthracenes /chrysenes							x	x	x
C2-benzo(a)anthracenes /chrysenes							x	x	x
C3-benzo(a)anthracenes /chrysenes								x	x
C4-benzo(a)anthracenes /chrysenes								x	x
C1-fluoranthenes/pyrenes							x	x	x
C2-fluoranthenes/pyrenes							x		
C1-fluorenes							x	x	x
C2-fluorenes							x	x	x
C3-fluorenes							x	x	x
C1-naphthalenes								x	x
C2-naphthalenes							x	x	x
C3-naphthalenes							x	x	x
C4-naphthalenes							x	x	x
C1-phenanthrenes/anthracenes							x	x	x
C2-phenanthrenes/anthracenes							x	x	x
C3-phenanthrenes/anthracenes							x	x	x
C4-phenanthrenes/anthracenes								x	x
Total Number of PAHs ^B	23	25	23	23	23	23	33 ^C	34	34
Number of data points	640	137	182	40	153	318	30	280	229

^A Benzo(b)fluoranthene and benzo(k)fluoranthene were measured together.

^B A specific C1-PAH was not included in the total if the C1 alkylated PAH series was measured.

For example, 1-methylnaphthalene was not included in the total if the C1-naphthalenes were measured.

^C For this dataset, the C1-Naphthalenes were not measured. As a result, the 1-methylnaphthalene and 2-methylnaphthalene were considered when determining the total number of PAHs.

Table 6-3. Teratogenic and carcinogenic effects of benzo(a)pyrene (BaP) and anthracene on freshwater and saltwater fishes. Measured concentrations of exposure are converted to sediment concentrations (C_{OC}) likely to result in the equivalent effect using EqP and SAR methodology.

Organism	Chemical	$\log_{10} K_{OW}$	$\log K_{OC}$	Measured C_d^a ($\mu\text{g/L}$)	C_d -derived C_{OC} ($\mu\text{g/g}_{OC}$)	Measured C_{ORG}^b ($\mu\text{g/g}$)	f_{Lipid}	C_L^b ($\mu\text{g/g Lipid}$)	C_L -derived C_{OC} ($\mu\text{g/g}_{OC}$)	References
TERATOGENIC EFFECTS										
<u>FRESHWATER</u>										
Fathead minnow eggs	Anthracene	4.53	4.46	-	-	8.8	0.06	147	219	Hall and Oris, 1991
Topminnows	BaP	6.11	6.00	>3.81 ^c (1,000)	>3810	9	0.06	150	256	Goddard et al., 1987
Rainbow trout eggs	BaP	6.11	6.00	0.21	210	1.9	0.05	38.6	66	Hannah et al., 1982 Hose et al., 1984
<u>SALTWATER</u>										
English sole eggs	BaP	6.11	6.00	-	-	157	0.03	5233 ^d	8,937 ^d	Hose et al., 1981
Sand sole eggs	BaP	6.11	6.00	0.10	100	2.1	0.03	70	120	Hose et al., 1982
Calif. grunion eggs	BaP	6.11	6.00	>3.81 (5)	>3810	1	0.03	33.3	57	Winkler et al., 1983
Calif. grunion eggs	BaP	6.11	6.00	>3.81 (24)	>3810	10.5	0.03	350	598	Winkler et al., 1983
Calif. grunion eggs	BaP	6.11	6.00	>3.81 ^c (869)	>3810	20.0	0.03	666	1,137	Winkler et al., 1983
CARCINOGENIC EFFECTS										
<u>FRESHWATER</u>										
Japanese medaka	BaP	6.11	6.00	>3.81 ^c (261)	>3840	-	-	-	-	Hawkins et al., 1988, 1990
guppy	BaP	6.11	6.00	>3.81 ^c (209)	>3840	-	-	-	-	Hawkins et al., 1988, 1990

If the concentration of BaP exceeded its solubility of 3.81 $\mu\text{g/L}$, the published concentration in water is listed in parenthesis with the solubility of 3.81 $\mu\text{g/L}$ listed above as the concentration of exposure. Therefore the maximum C_{OC} value for these exposures is 3840 $\mu\text{g BaP/g}_{OC}$.

Concentrations in eggs on a wet weight basis are converted to concentrations on a lipid basis using lipid concentrations (f_{Lipid}) from Table 1 in Kamler (1992).

Water concentrations of BaP were not stable throughout the duration of the experiment.

The solubility of BaP in water theoretically limits the maximum concentration in eggs to ~3,840 $\mu\text{g/g lipid}$ and in sediments to ~3,840 $\mu\text{g/g}_{OC}$, but metabolites of BaP will likely be included in radio-labeled quantification of total BaP equivalents.

Table 6-2. PAH measured in various sediment monitoring programs. See Di Toro and McGrath (2000) for data sources.

Parameter	NOAA	SFEI	San Diego	Southern California	NY/NJ REMAP ^A	Virginian EMAP ^B	Elliott Bay	Carolinian EMAP	Louisian EMAP
Acenaphthene	x	x	x	x	x	x	x	x	x
Acenaphthylene	x	x	x	x	x	x	x	x	x
Anthracene	x	x	x	x	x	x	x	x	x
Chrysene	x	x	x	x	x	x	x	x	x
Fluoranthene	x	x	x	x	x	x	x	x	x
Fluorene	x	x	x	x	x	x	x	x	x
naphthalene	x	x	x	x	x	x	x	x	x
phenanthrene	x	x	x	x	x	x	x	x	x
pyrene	x	x	x	x	x	x	x	x	x
Benzo(k)fluoranthene	x	x	x	x	x	x	x	x	x
Benzo(b)fluoranthene	x	x	x	x	x	x	x	x	x
Benzo(a)pyrene	x	x	x	x	x	x	x	x	x
Benzo(a)anthracene	x	x	x	x	x	x	x	x	x
Benzo(e)pyrene	x	x	x	x	x	x	x	x	x
Benzo(g,h,i)perylene	x	x	x	x	x	x	x	x	x
Dibenz(a,h)anthracene	x	x	x	x	x	x	x	x	x
2,6-dimethylnaphthalene	x	x	x	x	x	x	x	x	x
Indeno(1,2,3-cd)pyrene	x	x	x	x	x	x	x	x	x
1-methylnaphthalene	x	x	x	x	x	x	x	x	x
2-methylnaphthalene	x	x	x	x	x	x	x	x	x
perylene	x	x	x	x	x	x	x	x	x
1-methylphenanthrene	x	x	x	x	x	x	x	x	x
2,3,5-trimethylnaphthalene	x	x	x	x	x	x	x	x	x
2-methylantracene							x		
2-methylphenanthrene		x					x		
3,6-dimethylphenanthrene							x		
9-methylantracene		x					x		
9,10-dimethylantracene							x		
C1-benzo(a)anthracenes /chrysenes							x	x	x
C2-benzo(a)anthracenes /chrysenes							x	x	x
C3-benzo(a)anthracenes /chrysenes								x	x
C4-benzo(a)anthracenes /chrysenes								x	x
C1-fluoranthenes/pyrenes							x	x	x
C2-fluoranthenes/pyrenes							x		
C1-fluorenes							x	x	x
C2-fluorenes							x	x	x
C3-fluorenes							x	x	x
C1-naphthalenes								x	x
C2-naphthalenes							x	x	x
C3-naphthalenes							x	x	x
C4-naphthalenes							x	x	x
C1-phenanthrenes/anthracenes							x	x	x
C2-phenanthrenes/anthracenes							x	x	x
C3-phenanthrenes/anthracenes							x	x	x
C4-phenanthrenes/anthracenes								x	x
Total Number of PAHs ^B	23	25	23	23	23	23	33 ^C	34	34
Number of data points	640	137	182	40	153	318	30	280	229

^A Benzo(b)fluoranthene and benzo(k)fluoranthene were measured together.

^B A specific C1-PAH was not included in the total if the C1 alkylated PAH series was measured.

For example, 1-methylnaphthalene was not included in the total if the C1-naphthalenes were measured.

^C For this dataset, the C1-Naphthalenes were not measured. As a result, the 1-methylnaphthalene and 2-methylnaphthalene were considered when determining the total number of PAHs.

Table 6-3. Teratogenic and carcinogenic effects of benzo(a)pyrene (BaP) and anthracene on freshwater and saltwater fishes. Measured concentrations of exposure are converted to sediment concentrations (C_{OC}) likely to result in the equivalent effect using EqP and SAR methodology.

Organism	Chemical	$\log_{10} K_{OW}$	$\log K_{OC}$	Measured C_d^a ($\mu\text{g/L}$)	C_d -derived C_{OC} ($\mu\text{g/g}_{OC}$)	Measured C_{ORG}^b ($\mu\text{g/g}$)	f_{Lipid}	C_L^b ($\mu\text{g/g Lipid}$)	C_L -derived C_{OC} ($\mu\text{g/g}_{OC}$)	References
TERATOGENIC EFFECTS										
<u>FRESHWATER</u>										
Fathead minnow eggs	Anthracene	4.53	4.46	-	-	8.8	0.06	147	219	Hall and Oris, 1991
Topminnows	BaP	6.11	6.00	>3.81 ^c (1,000)	>3810	9	0.06	150	256	Goddard et al., 1987
Rainbow trout eggs	BaP	6.11	6.00	0.21	210	1.9	0.05	38.6	66	Hannah et al., 1982 Hose et al., 1984
<u>SALTWATER</u>										
English sole eggs	BaP	6.11	6.00	-	-	157	0.03	5233 ^d	8,937 ^d	Hose et al., 1981
Sand sole eggs	BaP	6.11	6.00	0.10	100	2.1	0.03	70	120	Hose et al., 1982
Calif. grunion eggs	BaP	6.11	6.00	>3.81 (5)	>3810	1	0.03	33.3	57	Winkler et al., 1983
Calif. grunion eggs	BaP	6.11	6.00	>3.81 (24)	>3810	10.5	0.03	350	598	Winkler et al., 1983
Calif. grunion eggs	BaP	6.11	6.00	>3.81 ^c (869)	>3810	20.0	0.03	666	1,137	Winkler et al., 1983
CARCINOGENIC EFFECTS										
<u>FRESHWATER</u>										
Japanese medaka	BaP	6.11	6.00	>3.81 ^c (261)	>3840	-	-	-	-	Hawkins et al., 1988, 1990
guppy	BaP	6.11	6.00	>3.81 ^c (209)	>3840	-	-	-	-	Hawkins et al., 1988, 1990

If the concentration of BaP exceeded its solubility of 3.81 $\mu\text{g/L}$, the published concentration in water is listed in parenthesis with the solubility of 3.81 $\mu\text{g/L}$ listed above as the concentration of exposure. Therefore the maximum C_{OC} value for these exposures is 3840 $\mu\text{g BaP/g}_{OC}$.

Concentrations in eggs on a wet weight basis are converted to concentrations on a lipid basis using lipid concentrations (f_{Lipid}) from Table 1 in Kamler (1992).

Water concentrations of BaP were not stable throughout the duration of the experiment.

The solubility of BaP in water theoretically limits the maximum concentration in eggs to ~3,840 $\mu\text{g/g lipid}$ and in sediments to ~3,840 $\mu\text{g/g}_{OC}$, but metabolites of BaP will likely be included in radio-labeled quantification of total BaP equivalents.

Appendix A. Individual datasets which comprise the acute lethality data base. Table from Di Toro et al. (2000).

Common Name, Scientific Name	Test Conditions			No. of Data Points ^c	References
	Test Duration (hr)	Method ^a	Concentration ^b		
<u>Freshwater</u>					
Paramecium, <i>Tetrahymena ellioti</i>	24	S	U	10(12)	Rogerson et al., 1983
Hydra, <i>Hydra oligactis</i>	48	S	U	5	Slooff et al., 1983
Snail, <i>Lymnae stagnalis</i>	48	S	U	5	Slooff et al., 1983
Cladocera ⁿ , <i>Daphnia cucullata</i>	48	S	U	5	Canton and Adema, 1978
Cladoceran, <i>Daphnia magna</i>	24	S	U	21(28)	LeBlanc, 1980a
Cladoceran, <i>Daphnia magna</i>	48	S	U	72(78)	Abernethy et al., 1988; U.S. EPA, 1978; Canton and Adema, 1978 Rogerson et al., 1983; Bringman and Kuhn, 1959; Eastman et al., 1984; Dill, 1980
Cladoceran, <i>Daphnia magna</i>	48	S	U	19	EG&G Bionomics, 1982; Thurston et al., 1985; Adema, 1978; Oris et al., 1991; Brooke, 1991; Millemann et al., 1984; Munkrittrick et al., 1991
Cladoceran, <i>Daphnia magna</i>	48	FT,R	M	1(2)	EG&G Bionomics, 1982; Brooke, 1994
Cladoceran, <i>Daphnia pulex</i>	48	S	M	(1)	Trucco et al., 1983
Cladoceran, <i>Daphnia pulex</i>	48	S	U	6	Canton and Adema, 1978; Passino and Smith, 1987

Common Name, Scientific Name	Test Conditions			No. of Data Points ^c	References
	Test Duration (hr)	Method ^a	Concentration ^b		
Brine shrimp, <i>Artemia salina</i>	24	S	N	32(34)	Abernethy et al., 1988; Abernethy et al., 1986
Crayfish, <i>Orconectes immunis</i>	96	FT	M	6	Thurston et al., 1985; Holcombe et al., 1987
Mosquito, <i>Aedes aegypti</i>	48	S	U	5	Slooff et al., 1983
Mosquito, <i>Culex pipiens</i>	48	S	U	5	Slooff et al., 1983
Midge, <i>Tanytarsus dissimilis</i>	48	S	M	9	Thurston et al., 1985; Call et al., 1983
Rainbow trout, <i>Oncorhynchus mykiss</i>	48	FT	M	7	Holcombe et al., 1987; Call et al., 1983
Rainbow trout, <i>Oncorhynchus mykiss</i>	24	FT	M	6	Call et al., 1983
Rainbow trout, <i>Oncorhynchus mykiss</i>	24	S	U	1(2)	Bently et al., 1975
Rainbow trout, <i>Oncorhynchus mykiss</i>	48	S	U	6	Slooff et al., 1983; Bently et al., 1975
Rainbow trout, <i>Oncorhynchus mykiss</i>	96	FT	M	22	Thurston et al., 1985; Call et al., 1983; Holcombe et al., 1987; Call et al., 1986; DeGraeve et al., 1982; Hodson et al., 1988
Rainbow trout, <i>Oncorhynchus mykiss</i>	96	S	M	1	Horne et al., 1983
Rainbow trout, <i>Oncorhynchus mykiss</i>	96	S	U	1	Bently et al., 1975

Appendix A. Individual datasets which comprise the acute lethality data base. Table from Di Toro et al. (2000).

Common Name, Scientific Name	Test Conditions			No. of Data Points ^c	References
	Test Duration (hr)	Method ^a	Concentration ^b		
<u>Freshwater</u>					
Paramecium, <i>Tetrahymena ellioti</i>	24	S	U	10(12)	Rogerson et al., 1983
Hydra, <i>Hydra oligactis</i>	48	S	U	5	Slooff et al., 1983
Snail, <i>Lymnae stagnalis</i>	48	S	U	5	Slooff et al., 1983
Cladocera ⁿ , <i>Daphnia cucullata</i>	48	S	U	5	Canton and Adema, 1978
Cladoceran, <i>Daphnia magna</i>	24	S	U	21(28)	LeBlanc, 1980a
Cladoceran, <i>Daphnia magna</i>	48	S	U	72(78)	Abernethy et al., 1988; U.S. EPA, 1978; Canton and Adema, 1978 Rogerson et al., 1983; Bringman and Kuhn, 1959; Eastman et al., 1984; Dill, 1980
Cladoceran, <i>Daphnia magna</i>	48	S	U	19	EG&G Bionomics, 1982; Thurston et al., 1985; Adema, 1978; Oris et al., 1991; Brooke, 1991; Millemann et al., 1984; Munkrittrick et al., 1991
Cladoceran, <i>Daphnia magna</i>	48	FT,R	M	1(2)	EG&G Bionomics, 1982; Brooke, 1994
Cladoceran, <i>Daphnia pulex</i>	48	S	M	(1)	Trucco et al., 1983
Cladoceran, <i>Daphnia pulex</i>	48	S	U	6	Canton and Adema, 1978; Passino and Smith, 1987

Common Name, Scientific Name	Test Conditions				References
	Test Duration (hr)	Method ^a	Concentration ^b	No. of Data Points ^c	
Brine shrimp, <i>Artemia salina</i>	24	S	N	32(34)	Abernethy et al., 1988; Abernethy et al., 1986
Crayfish, <i>Orconectes immunis</i>	96	FT	M	6	Thurston et al., 1985; Holcombe et al., 1987
Mosquito, <i>Aedes aegypti</i>	48	S	U	5	Slooff et al., 1983
Mosquito, <i>Culex pipiens</i>	48	S	U	5	Slooff et al., 1983
Midge, <i>Tanytarsus dissimilis</i>	48	S	M	9	Thurston et al., 1985; Call et al., 1983
Rainbow trout, <i>Oncorhynchus mykiss</i>	48	FT	M	7	Holcombe et al., 1987; Call et al., 1983
Rainbow trout, <i>Oncorhynchus mykiss</i>	24	FT	M	6	Call et al., 1983
Rainbow trout, <i>Oncorhynchus mykiss</i>	24	S	U	1(2)	Bently et al., 1975
Rainbow trout, <i>Oncorhynchus mykiss</i>	48	S	U	6	Slooff et al., 1983; Bently et al., 1975
Rainbow trout, <i>Oncorhynchus mykiss</i>	96	FT	M	22	Thurston et al., 1985; Call et al., 1983; Holcombe et al., 1987; Call et al., 1986; DeGraeve et al., 1982; Hodson et al., 1988
Rainbow trout, <i>Oncorhynchus mykiss</i>	96	S	M	1	Horne et al., 1983
Rainbow trout, <i>Oncorhynchus mykiss</i>	96	S	U	1	Bently et al., 1975

Common Name, Scientific Name	Test Conditions				References
	Test Duration (hr)	Method ^a	Concentration ^b	No. of Data Points ^c	
Bleak, <i>Alburnus alburnus</i>	96	S	I	7	Bengtsson et al., 1984
Goldfish, <i>Carasius auratus</i>	24	S	M	26(28)	Bridie et al., 1979
Goldfish, <i>Carasius auratus</i>	24	S	U	5(6)	Pickering and Henderson, 1966
Goldfish, <i>Carasius auratus</i>	24	FT	M	1(2)	Brenniman et al., 1976
Goldfish, <i>Carasius auratus</i>	96	S	U	4	Pickering and Henderson, 1966
Goldfish, <i>Carasius auratus</i>	96	FT	M	1(2)	Brenniman et al., 1976
Goldfish, <i>Carasius auratus</i>	48	S	U	5(6)	Pickering and Henderson, 1966
Goldfish, <i>Carasius auratus</i>	48	FT	M	1(2)	Brenniman et al., 1976
Golden orfe, <i>Leuciscus idus melanotus</i>	24	S	I(ns)	26	Juhnke and Ludemann, 1978
Fathead minnow, <i>Pimephales promelas</i>	24	S	U	6	Pickering and Henderson, 1966
Fathead minnow, <i>Pimephales promelas</i>	24	FT	M	8	Ahmad et al., 1984
Fathead minnow, <i>Pimephales promelas</i>	48	S	U	11	Pickering and Henderson, 1966

Common Name, Scientific Name	Test Conditions				References
	Test Duration (hr)	Method ^a	Concentration ^b	No. of Data Points ^c	
Fathead minnow, <i>Pimephales promelas</i>	48	FT	M	8	Ahmad et al., 1984
Fathead minnow, <i>Pimephales promelas</i>	96	FT	M	141(146)	Veith et al., 1983; Thurston et al., 1985; Holcombe et al., 1987; Ahmad et al., 1984; Dill, 1980; DeGraeve et al., 1982; Alexander et al., 1978; Broderius and Kahl, 1985; Cairns and Nebeker, 1982; Hall et al., 1989; Hall et al., 1984; Call et al., 1985; CLSES, 1984; CLSES, 1985; CLSES, 1986; CLSES, 1988; CLSES, 1990; Kimball, 1978
Fathead minnow, <i>Pimephales promelas</i>	96	S	M	3(4)	Bridie et al., 1979; EG&G Bionomics, 1982; Gendussa, 1990; Horne et al., 1983
Fathead minnow, <i>Pimephales promelas</i>	96	R	U	1	Academy Natural Sci., 1981
Fathead minnow, <i>Pimephales promelas</i>	96	S	U	4	Pickering and Henderson, 1966
Channel catfish, <i>Ictalurus punctatus</i>	96	FT,S	M	7	Thurston et al., 1985; Holcombe et al., 1983; Gendussa, 1990
Medaka, <i>Oryzias latipes</i>	48	S	U	4(5)	Slooff et al., 1983
American flagfish, <i>Jordanella floridae</i>	24	FT	M	6	Smith et al., 1991
American flagfish, <i>Jordanella floridae</i>	48	FT	M	6	Smith et al., 1991
American flagfish, <i>Jordanella floridae</i>	96	FT	M	6	Smith et al., 1991

Common Name, Scientific Name	Test Conditions			No. of Data Points ^c	References
	Test Duration (hr)	Method ^a	Concentration ^b		
Mosquitofish, <i>Gambusia affinis</i>	24	S	U	(3)	Thurston et al., 1985
Mosquitofish, <i>Gambusia affinis</i>	48	S	U	(3)	Thurston et al., 1985
Mosquitofish, <i>Gambusia affinis</i>	96	FT	M	5(6)	Thurston et al., 1985; Wallen et al., 1957
Mosquitofish, <i>Gambusia affinis</i>	96	S	U	3	Wallen et al., 1957
Guppy, <i>Poecilia reticulata</i>	24	S	U	(1)	Pickering and Henderson, 1966
Guppy, <i>Poecilia reticulata</i>	48	S	U	10(11)	Slooff et al., 1983; Pickering and Henderson, 1966
Guppy, <i>Poecilia reticulata</i>	96	S	U	4	Slooff et al., 1983
Bluegill, <i>Lepomis macrochirus</i>	24	S	U	18(19)	Pickering and Henderson, 1966; Buccafusco et al., 1981; Bently et al., 1975
Bluegill, <i>Lepomis macrochirus</i>	24	FT	M	1	Call et al., 1983
Bluegill, <i>Lepomis macrochirus</i>	48	FT	M	1	Call et al., 1983
Bluegill, <i>Lepomis macrochirus</i>	48	S	U	6(7)	Pickering and Henderson, 1966; Bently et al., 1975
Bluegill, <i>Lepomis macrochirus</i>	96	FT	M	8	Thurston et al., 1985; Bently et al., 1975; Call et al., 1983; Holcombe et al., 1987

Common Name, Scientific Name	Test Conditions			No. of Data Points ^c	References
	Test Duration (hr)	Method ^a	Concentration ^b		
Bluegill, <i>Lepomis macrochirus</i>	96	S	U	36(40)	Pickering and Henderson, 1966; U.S. EPA, 1978; LeBlanc, 1980b; ; Buccafusco et al., 1981; Bently et al., 1975; Dawson et al., 1977. 1
Tadpole, <i>Rana catesbeiana</i>	96	FT	M	5	Thurston et al., 1985
Clawed toad, <i>Xenopus laevis</i>	48	S	U	5	Slooff and Baerselman, 1980
Mexican axolotl, <i>Ambystoma mexicanum</i>	48	S	U	5	Slooff and Baerselman, 1980
<u>Saltwater</u>					
Annelid worm, <i>Neanthes arenaceodentata</i>	96	S	U	4(5)	Horne et al., 1983; Rossi and Neff, 1978
Annelid worm, <i>Neanthes arenaceodentata</i>	96	R	U	(1)	Thursby et al., 1989a
Copepod, <i>Nitocra spinipes</i>	96	S	I	6	Bengtsson et al., 1984
Amphipod, <i>Leptocheirus plumulosus</i>	96	FT	M	4	Swartz, 1991a; Champlin and Poucher, 1992a; Boese et al., 1997
Mysid, <i>Americamysis bahia</i>	96	S	U	20(23)	U.S. EPA, 1978; Champlin and Poucher, 1992a; Zarogian et al., 1985
Mysid, <i>Americamysis bahia</i>	96	S	M	1	EG&G Bionomics, 1982
Mysid, <i>Americamysis bahia</i>	96	R	U	1 8(9)	Thursby et al., 1989b

Common Name, Scientific Name	Test Conditions				References
	Test Duration (hr)	Method ^a	Concentration ^b	No. of Data Points ^c	
Mysid, <i>Americamysis bahia</i>	96	FT	M	8(9)	Battelle, 1987; Champlin and Poucher, 1992a; Horne et al., 1983; EG&G Bionomics, 1978; U.S. EPA, 1978; Kuhn and Lussier, 1987; Thursby, 1991b
Grass shrimp, <i>Palaemonetes pugio</i>	96	R	U	2	Battelle, 1987; Thursby et al., 1989a
Grass shrimp, <i>Palaemonetes pugio</i>	96	S	U	4	Champlin and Poucher, 1992a; Horne et al., 1983; Thursby, 1991b; Tatem et al., 1978
Grass shrimp, <i>Palaemonetes pugio</i>	96	FT	M	1	Battelle, 1987
Grass shrimp, <i>Palaemonetes pugio</i>	96	S	M	1	Tatem, 1977
Crab, <i>Portunus pelagicus</i>	96	S	M	4	Mortimer and Connell, 1994
Inland silverside, <i>Menidia beryllina</i>	96	R	U	1	Thursby et al., 1989a
Inland silverside, <i>Menidia beryllina</i>	96	S	U	7(8)	Champlin and Poucher, 1992a; Dawson et al., 1977; Horne et al., 1983
Sheepshead minnow, <i>Cyprinodon variegatus</i>	24	S	U	7(8)	Heitmuller et al., 1981
Sheepshead minnow, <i>Cyprinodon variegatus</i>	48	S	U	11(12)	Heitmuller et al., 1981
Sheepshead minnow, <i>Cyprinodon variegatus</i>	96	S	U	13(15)	Heitmuller et al., 1981; U.S. EPA, 1978

Common Name, Scientific Name	Test Conditions				References
	Test Duration (hr)	Method ^a	Concentration ^b	No. of Data Points ^c	
Sheepshead minnow, <i>Cyprinodon variegatus</i>	96	FT	M	2	Ward et al., 1981; Battelle, 1987
Total Data Points				736 (796)	

^aMethod: S=static, FT=flow-through, R=renewal

^bConcentration: U=unmeasured (nominal), M=chemical measured, I=initial

^cNumber of data points used; ()=number of data before screening for concentration > solubility and outliers.

Appendix B. Chemicals which comprise the acute toxicity database for narcosis chemicals in Section 2 of this document. Table from Di Toro et al. (2000).

Chemical	CAS ^A	Class ^B	K_{ow} ^C	MW ^D	MV ^E	S^F
triethylene glycol	112276	ao	-1.48	150.17	131	-
methanol	67561	ao	-0.715	32.04	41.0	13.5
2,4-pentanedione*	123546	k	-0.509	100.12	100	7.87
ethanol	64175	ao	-0.234	46.07	59.0	11.9
acetone	67641	k	-0.157	58.08	74.0	13.71
2-chloroethanol*	107073	ao	-0.048	80.51	65.0	9.09
2-(2-ethoxyethoxy)ethanol	111900	ao	0.011	134.17	111	-
1-chloro-2-propanol*	127004	ao	0.156	94.54	84.0	44.8
1,3-dichloro-2-propanol*	96231	ao	0.165	128.99	91.0	6.30
2-methyl-2,4-pentanediol	107415	ao	0.246	118.17	120	43.0
2-butanone	78933	k	0.316	72.11	90.0	2.81
2-propanol	67630	ao	0.341	60.10	77.0	13.6
3-chloro-1-propanol*	627305	ao	0.363	94.54	82.0	2.00
1-propanol	71238	ao	0.399	60.10	75.0	11.2
cyclopentanone	120923	k	0.453	84.12	89.0	1.11
2-methyl-2-propanol	75650	ao	0.663	74.12	95.0	16.5
methyl chloride	74873	al,ha	0.677	50.49	56.0	0.0666
2-butanol	78922	ao	0.717	74.12	93.0	14.9
methyl bromide*	74839	al,ha	0.791	94.94	57.0	0.154
3-methyl-2-butanone	563804	k	0.792	86.13	108	1.32
2,3-dibromopropanol*	96139	ao	0.819	217.90	96.0	5.97
cyclohexanone	108941	k	0.827	98.14	103	0.445
cyclopentanol	96413	ao	0.849	86.13	89.0	5.19
2-methyl-1-propanol	78831	ao	0.858	74.12	93.0	10.6
4-methyl-3-pente-2-one	141797	k	0.867	98.14	118	2.68
2-pentanone	107879	k	0.877	86.13	107	1.03
1-butanol	71363	ao	0.946	74.12	92.0	3.03
3-pentanone	96220	k	0.954	86.13	108	0.849

Chemical	CAS ^A	Class ^B	K _{OW} ^C	MW ^D	MV ^E	S ^F
2-methyl-2-butanol	75854	ao	1.03	88.15	110	1.62
2-n-butoxyethanol	111762	ao	1.05	118.17	131	8.78
diethyleneglycolmono-n-butylether	112345	et	1.09	162.23	170	40.0
3,3-dimethyl-2-butanone	75978	k	1.09	100.16	125	0.954
diethyl ether	60297	et	1.15	74.122	105	1.16
4-methoxy-4-methyl-2-pentane	107700	k	1.17	130.19	143	41.5
4-methyl-2-pentanone	108101	k	1.17	100.16	124	0.862
dichloromethane	75092	al,ha	1.18	84.93	65.0	0.211
t-butylmethyl ether	1634044	et	1.20	88.149	122	9.04
cyclohexanol	108930	ao	1.29	100.16	103	1.61
2-hexanone	591786	k	1.29	100.16	124	0.598
1,2-dichloroethane	107062	al,ha	1.40	98.96	79.0	0.114
1-pentanol	71410	ao	1.49	88.15	109	0.581
3-methyl-3-pentanol	77747	ao	1.49	102.18	125	3.79
2-phenoxyethanol	122996	ao	1.50	138.17	122	0.173
2,2,2-trichloroethanol	115208	ao	1.61	149.4	93.0	48.4
4-methyl-2-pentanol	108112	ao	1.66	102.18	126	2.25
3-hexanol	623370	ao	1.66	102.18	125	2.18
2-heptanone	110430	ke	1.67	114.19	141	0.312
5-methyl-2-hexanone	110123	ke	1.68	114.19	141	0.271
2,4-dimethyl-3-pentanol	600362	ao	1.78	116.2	140	3.05
6-methyl-5-heptene-2-one	110930	ke	1.82	126.2	151	0.487
2-hexanol	626937	ao	1.83	102.18	126	1.13
1,3-dichloropropane	142289	al,ha	1.84	112.99	97.0	0.0363
1,2-dichloropropane	78875	al,ha	1.86	112.99	99.0	0.0342
diisopropyl ether	108203	et	1.87	102.18	138	0.0918
chloroform	67663	al,ha	1.91	119.38	81.0	0.0319
1,1,2-trichloroethane	79005	al,ha	1.91	133.4	94.0	0.0369
1,4-dimethoxybenzene	150787	ar	1.95	138.165	132	0.0250
2,6-dimethoxytoluene	5673074	ar	1.99	152.19	147	0.0283

Chemical	CAS ^A	Class ^B	K _{ow} ^C	MW ^D	MV ^E	S ^F
benzene	71432	ar	2.00	78.11	89.0	0.0260
1-hexanol	111273	ao	2.02	102.18	125	0.159
2-octanone	111137	ke	2.02	128.21	157	0.111
1-chloro-3-bromopropane	109706	al,ha	2.04	157.44	100	0.0184
5-methyl-3-heptanone	541855	ke	2.05	128.21	156	0.111
anisole	100663	ar	2.06	108.14	111	0.0148
2,6-dimethyl-2,5-heptadiene	504201	ke	2.07	138.21	164	0.0171
1,2-dichloroethylene	156605	al,ha	2.10	96.94	81.0	0.0202
1,2,3-trichloropropane	96184	al,ha	2.13	147.43	107	0.0177
1,1-dichloroethylene	75354	al,ha	2.19	96.94	81.0	0.0141
1,3-dibromopropane*	109648	al,ha	2.24	201.9	103	0.00930
bromoform	75252	al,ha	2.25	252.73	88.0	0.00650
1,1,2,2-tetrachloroethane	79345	al,ha	2.31	167.85	106	0.0181
1,4-dichlorobutane	110565	al,ha	2.33	127.01	113	0.00990
1,1-dichloropropane	78999	al,ha	2.36	112.99	101	0.00790
2-nonanone	821556	ke	2.38	142.24	174	0.0801
1,1,1-trichloroethane	71556	al,ha	2.38	133.4	101	0.00662
1,1,1,2-tetrachloroethane	630206	al,ha	2.43	167.85	110	0.0050
5-nonanone	502567	ke	2.44	142.24	174	0.0740
1-heptanol	111706	ao	2.57	116.2	142	0.0487
chlorobenzene	108907	ar,ha	2.58	112.56	102	0.00320
2-ethyl-1-hexanol	104767	ao	2.58	130.23	155	0.132
bicyclo(2,2,1)hepta-2,5-diene	121460	al	2.60	92.14	102	0.00490
toluene	108883	ar	2.62	92.14	107	0.00600
styrene	100425	ar	2.72	104.15	116	0.00550
tetrachloromethane	56235	al,ha	2.73	153.82	97.0	0.00248
2-decanone	693549	ke	2.73	156.27	190	0.0599
bromobenzene	108861	ar,ha	2.75	157.01	106	0.00196
cyclopentane	278923	al	2.76	70.134	95.0	0.00260
1,5-dichloropentane	628762	al,ha	2.76	141.04	130	0.00286

Chemical	CAS ^A	Class ^B	K _{ow} ^C	MW ^D	MV ^E	S ^F
1,3,5-cycloheptatriene	544252	al	2.77	92.14	104	0.00377
trichloroethylene	79016	al,ha	2.81	131.39	90.0	0.00360
di-n-butyl ether	142961	et	2.89	130.23	170	0.00614
t-1,2-dichlorocyclohexane	822866	al,ha	2.90	153.05	128	0.00162
pentachloroethane	76017	al,ha	2.95	202.29	121	0.00111
2,4-hexadiene	592461	al	2.98	82.145	115	0.00237
butylphenyl ether	1126790	et	3.00	150.22	160	0.000790
benzophenone	119619	ke	3.05	182.22	163	0.000480
ethylbenzene	100414	ar	3.06	106.17	123	0.00219
2,3-dimethyl-1,3-butadiene	513815	al	3.06	82.145	121	0.00162
2-undecanone	112129	ke	3.08	170.29	207	0.0459
1-octanol	118875	ao	3.10	130.23	158	0.0161
3-chlorotoluene	108418	ar,ha	3.12	126.59	118	0.000834
4-chlorotoluene	106434	ar,ha	3.13	126.59	118	0.000817
o-xylene	95476	ar	3.13	106.17	121	0.00191
m-xylene	108383	ar	3.19	106.17	124	0.00154
p-xylene	106423	ar	3.21	106.17	124	0.00146
1,4-dichlorobenzene	106467	ar,ha	3.24	147.00	113	0.000581
3,5,5-trimethyl-1-hexanol	3452979	ao	3.29	144.26	172	0.0117
1,2-dichlorobenzene	95501	ar,ha	3.31	147.00	113	0.000507
1,3-dichlorobenzene	541731	ar,ha	3.31	147.00	115	0.000524
napthalene	91203	pah	3.36	128.17	125	0.00110
cyclohexane	110827	al	3.38	84.16	109	0.000919
tetrachloroethylene	127184	al,ha	3.38	165.83	99.0	0.000710

Chemical	CAS ^A	Class ^B	K _{ow} ^C	MW ^D	MV ^E	S ^F
2-dodecanone	6175491	ke	3.43	184.32	223	0.0357
cumene	98828	ar	3.49	120.19	140	0.000762
pentane	109660	al	3.50	72.15	116	0.000592
1,2-dibromobenzene	585539	ar,ha	3.56	235.92	119	0.000196
1,5-cyclooctadiene	111784	al	3.61	108.18	130	0.000386
1-nonanol	143088	ao	3.63	144.26	175	0.00552
1,2,4-trimethylbenzene	95636	ar	3.65	120.19	138	0.000487
n-propylbenzene	103651	ar	3.67	120.19	140	0.000467
dipentyl ether	693652	et	3.69	158.28	202	0.000757
1,3,5-trimethylbenzene	108678	ar	3.69	120.19	140	0.000414
hexachloroethane	67721	al,ha	3.73	236.74	132	0.0000936
2,4-dichlorotoluene	95738	ar,ha	3.79	161.03	129	0.000457
1-methylnaphthalene	90120	pah	3.84	142.20	140	0.000280
2-methylnaphthalene	91576	pah	3.86	142.20	141	0.000270
2-chloronaphthalene	91587	pah,ha	3.88	162.62	136	0.000100
1-chloronaphthalene	90131	pah,ha	3.88	162.62	136	0.000100
3,4-dichlorotoluene	95750	ar,ha	3.88	161.03	129	0.000120
biphenyl	92524	ar	3.91	154.21	150	0.000216
1,3,5-trichlorobenzene	108703	ar,ha	3.97	181.45	125	0.0000933
1,2,3-trichlorobenzene	87616	ar,ha	3.98	181.45	124	0.0000870
1,2,4-trichlorobenzene	120821	ar,ha	4.00	181.45	126	0.0000886

Chemical	CAS ^A	Class ^B	K _{ow} ^C	MW ^D	MV ^E	S ^F
acenaphthene	83329	pah	4.01	154.21	140	0.000100
2,5-dimethyl-2,4-hexadiene	764136	al	4.10	110.20	146	0.000133
methyl cyclohexane	108872	al	4.10	98.19	128	0.000155
1,2,4,5-tetramethylbenzene	95932	ar	4.11	134.22	152	0.000159
hexane	110543	al	4.12	86.18	132	0.000131
1,3-diethylbenzene	141935	ar	4.17	134.22	156	0.000135
1-decanol	112301	ao	4.19	158.28	192	0.00181
p-tert-butyltoluene	98511	ar	4.26	148.25	173	0.0000995
diphenylether	101848	et	4.36	170.21	152	0.0000595
amylbenzene	538681	ar	4.52	148.25	173	0.0000502
phenanthrene	85018	pah	4.57	178.23	161	0.0000340
1,2,4,5-tetrachlorobenzene	95943	ar,ha	4.64	215.89	136	0.0000151
1,2,3,4-tetrachlorobenzene	634662	ar,ha	4.64	215.89	136	0.0000145
1,2,3,5-tetrachlorobenzene	634902	ar,ha	4.64	215.89	136	0.0000148
1-undecanol	112425	ao	4.70	172.31	207	0.000640
pyrene	129000	pah	4.92	202.26	182	0.0000120
9-methylanthracene	779022	pah	5.01	192.26	175	0.00000980
fluoranthene	206440	pah	5.08	202.26	197	0.0000102
1-dodecanol	112538	ao	5.20	186.34	223	0.000238
pentachlorobenzene	608935	ar,ha	5.32	250.34	147	0.00000218
octane*	111659	al	5.34	114.23	164	0.00000625

Chemical	CAS ^A	Class ^B	K _{ow} ^C	MW ^D	MV ^E	S ^F
1-tridecanol*	112709	ao	5.75	200.36	224	0.0000793
decane*	124185	al	6.56	142.28	229	0.000000300

*Chemical is not included: LC50 > S.

^ACAS=Chemical abstract number

^BClass: ao=alcohol, ar=aromatic, ha=halogenated, et=ether, al=aliphatic, ke=ketone, pah=PAH

^CK_{ow}=log₁₀(K_{ow});

^DMW=molecular weight (gm/mol);

^EV=molar volume (cm³/mol);

^FS=aqueous solubility(mol/L)

Appendix C. Summary of data on the acute toxicity of PAHs to freshwater and saltwater species and the derivation of genus mean acute values.

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^A	HABITAT ^B	PAH TESTED (CAS #)	LOG K _{OW} ^C	METHOD ^D	CONCENTRATION ^E	LC50/EC50 ^F (μg/L)	LC50/EC50 ^F (μmol/L)	PAH SPECIFIC SMAV ^H (μmol/L)	K _{OW} NORMALIZED PAH SPECIFIC SMAV ^I (μmol/g _{OC})	SPECIES SMAV ^J (μmol/g _{OC})	GMVAV ^K (μmol/g _{OC})	REFERENCES
FRESHWATER													
Hydra, <i>Hydra americana</i>	J	W,E	fluoranthene (206-44-0)	5.08	FT	M	70	0.346	0.346	22.1	22.1	-	Spehar et al., 1999
Hydra, <i>Hydra sp.</i>	X	W,E	phenanthrene (85-01-8)	4.57	FT	M	96	0.539	0.539	11.2	11.2	15.5	Call et al., 1986
Annelid, <i>Lumbriculus variegatus</i>	X	I	phenanthrene (85-01-8)	4.57	FT	M	>419	>2.35	>2.35	>49.0	-	-	Call et al., 1986
Annelid, <i>Lumbriculus variegatus</i>	A	I	fluoranthene (206-44-0)	5.08	FT	M	>178	>0.880	>0.880	>56	>52.4	>52.4	Spehar et al., 1999
Snail, <i>Mudalia potosensis</i>	X	E	fluorene (86-73-7)	4.21	S	U	>1900 ^Q (5600)	>11.4	>11.4	>108	>108	>108	Finger et al., 1985
Snail, <i>Aplexa hypnorum</i>	X	E	acenaphthene (83-32-9)	4.01	FT	M	>2040	>13.2	>13.2	>81.8	>81.8	>81.8	Holcömbe et al., 1983
Snail, <i>Physa heterostrophia</i>	X	E	fluoranthene (206-44-0)	5.08	S	U	137	0.677	0.677	43.2	43.2	43.2	Horne and Oblad, 1983
Snail, <i>Physella virgata</i>	A	E	fluoranthene (206-44-0)	5.08	FT	M	>178	>0.880	>0.880	>56	>56	>56	Spehar et al., 1999
Cladoceran, <i>Daphnia magna</i>	X	W	naphthalene (91-20-3)	3.36	S	U	8570	66.9	-	-	-	-	U.S. EPA, 1978
Cladoceran, <i>Daphnia magna</i>	J	W	naphthalene (91-20-3)	3.36	S	U	4723	36.9	-	-	-	-	Abernethy et al., 1986
Cladoceran, <i>Daphnia magna</i>	X	W	naphthalene (91-20-3)	3.36	S	M	2160	16.9	34.6	51.0	-	-	Millemann et al., 1984
Cladoceran, <i>Daphnia magna</i>	J	W	1-methyl naphthalene (90-12-0)	3.84	S	U	1420	9.99	9.99	42.2	-	-	Abernethy et al., 1986

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^A	HABITAT ^B	PAH TESTED (CAS #)	LOG K _{ow} ^C	METHOD ^D	CONCENTRATION ^E	LC50/EC50 ^F (μg/L)	LC50/EC50 ^F (μmol/L)	PAH SPECIFIC SMAV ^H (μmol/L)	K _{ow} NORMALIZED PAH SPECIFIC SMAV ^I (μmol/g _{oc})	SPECIES SMAV ^I (μmol/g _{oc})	GMAV ^K (μmol/g _{oc})	REFERENCES
Cladoceran, <i>Daphnia magna</i>	J	W	2-methyl naphthalene (91-57-6)	3.86	S	U	1491	10.5	10.5	46.3	-	-	Abernethy et al., 1986
Cladoceran, <i>Daphnia magna</i>	X	W	acenaphthene (83-32-9)	4.01	S	U	3450	22.4	-	-	-	-	Randall and Knopp, 1980
Cladoceran, <i>Daphnia magna</i>	X	W	acenaphthene (83-32-9)	4.01	S	U	>3800 (41000)	>24.6	-	-	-	-	LeBlanc, 1980a
Cladoceran, <i>Daphnia magna</i>	X	W	acenaphthene (83-32-9)	4.01	S	M	320	2.08	-	-	-	-	EG&G Bionomics, 1982
Cladoceran, <i>Daphnia magna</i>	X	W	acenaphthene (83-32-9)	4.01	S	M	1300	8.43	-	-	-	-	EG&G Bionomics, 1982
Cladoceran, <i>Daphnia magna</i>	X	W	acenaphthene (83-32-9)	4.01	FT	M	120	0.778	0.778	4.80	-	-	EG&G Bionomics, 1982
Cladoceran, <i>Daphnia magna</i>	X	W	fluorene (86-73-7)	4.21	S	U	430	2.59	2.59	24.5	-	-	Finger et al., 1985
Cladoceran, <i>Daphnia magna</i>	J	W	phenanthrene (85-01-8)	4.57	S	U	207	1.16	-	-	-	-	Abernethy et al., 1986
Cladoceran, <i>Daphnia magna</i>	X	W	phenanthrene (85-01-8)	4.57	S	U	843	4.73	-	-	-	-	Eastmond et al., 1984
Cladoceran, <i>Daphnia magna</i>	Neonate	W	phenanthrene (85-01-8)	4.57	S	M	700	3.93	-	-	-	-	Millemann et al., 1984
Cladoceran, <i>Daphnia magna</i>	Neonate	W	phenanthrene (85-01-8)	4.57	S,R	M	212	1.19	-	-	-	-	Brooke, 1994
Cladoceran, <i>Daphnia magna</i>	Neonate	W	phenanthrene (85-01-8)	4.57	FT	M	230	1.29	-	-	-	-	Brooke, 1993
Cladoceran, <i>Daphnia magna</i>	X	W	phenanthrene (85-01-8)	4.57	FT	M	117	0.656	0.920	19.2	-	-	Call et al., 1986

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^A	HABITAT ^B	PAH TESTED (CAS #)	LOG K _{ow} ^C	METHOD ^D	CONCENTRATION ^E	LC50/EC50 ^F (μg/L)	LC50/EC50 ^F (μmol/L)	PAH SPECIFIC SMAV ^H (μmol/L)	K _{ow} NORMALIZED PAH SPECIFIC SMAV ^I (μmol/g _{oc})	SPECIES SMAV ^I (μmol/g _{oc})	GMAV ^K (μmol/g _{oc})	REFERENCES
Cladoceran, <i>Daphnia magna</i>	J	W	pyrene (129-00-0)	4.92	S	U	90.9	0.45	0.45	20.1	-	-	Abernethy et al., 1986
Cladoceran, <i>Daphnia magna</i>	J	W	9-methyl anthracene (779-02-2)	5.01	S	U	124.8	0.65	0.65	34.9	-	-	Abernethy et al., 1986
Cladoceran, <i>Daphnia magna</i>	J	W	fluoranthene (206-44-0)	5.08	S	U	>260 (320000)	>1.29	-	-	-	-	LeBlanc, 1980a
Cladoceran, <i>Daphnia magna</i>	J	W	fluoranthene (206-44-0)	5.08	S	M	45	0.222	-	-	-	-	Oris et al., 1991
Cladoceran, <i>Daphnia magna</i>	J	W	fluoranthene (206-44-0)	5.08	R	M	117	0.578	-	-	-	-	Spehar et al., 1999
Cladoceran, <i>Daphnia magna</i>	X	W	fluoranthene (206-44-0)	5.08	S	M	105.7	0.523	0.407	25.9	25.2	-	Suedel and Rodgers, 1996
Cladoceran, <i>Daphnia pulex</i>	X	W	naphthalene (91-20-3)	3.36	S	U	4663	36.4	36.4	54.0	-	-	Smith et al., 1988
Cladoceran, <i>Daphnia pulex</i>	X	W	fluorene (86-73-7)	4.21	S	U	212	1.27	1.27	12.1	-	-	Smith et al., 1988
Cladoceran, <i>Daphnia pulex</i>	X	W	1,3-dimethyl naphthalene (575-41-7)	4.37	S	U	767	4.92	4.92	66	-	-	Smith et al., 1988
Cladoceran, <i>Daphnia pulex</i>	X	W	2,6-dimethyl naphthalene (581-42-0)	4.37	S	U	193	1.24	1.24	16.8	-	-	Smith et al., 1988
Cladoceran, <i>Daphnia pulex</i>	X	W	anthracene (120-12-7)	4.53	S	U	>45 (754)	>0.25	>0.25	>4.9 ^L	-	-	Smith et al., 1988
Cladoceran, <i>Daphnia pulex</i>	Neonate	W	phenanthrene (85-01-8)	4.57	S	U	734	4.12	-	-	-	-	Passino and Smith, 1987

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^A	HABITAT ^B	PAH TESTED (CAS #)	LOG K _{ow} ^C	METHOD ^D	CONCENTRATION ^E	LC50/EC50 ^F (μg/L)	LC50/EC50 ^F (μmol/L)	PAH SPECIFIC SMAV ^H (μmol/L)	K _{ow} NORMALIZED PAH SPECIFIC SMAV ^I (μmol/g _{oc})	SPECIES SMAV ^I (μmol/g _{oc})	GMAV ^K (μmol/g _{oc})	REFERENCES
Cladoceran, <i>Daphnia pulex</i>	X	W	phenanthrene (85-01-8)	4.57	S	U	>1100 (>1150)	>6.17	-	-	-	-	Geiger and Buikema, 1981, 1982
Cladoceran, <i>Daphnia pulex</i>	X	W	phenanthrene (85-01-8)	4.57	S	U	350	1.96	-	-	-	-	Smith et al., 1988
Cladoceran, <i>Daphnia pulex</i>	X	W	phenanthrene (85-01-8)	4.57	S	M	100	0.56	1.66	34.6	-	-	Trucco et al., 1983
Cladoceran, <i>Daphnia pulex</i>	X	W	2-methyl anthracene (613-12-7)	4.99	S	U	>30 (96)	>0.156	>0.156	>8.1 ^L	30.2	27.6	Smith et al., 1988
Amphipod, <i>Gammarus minus</i>	X	E	acenaphthene (83-32-9)	4.01	S	U	460	3.0	3.0	18.4	-	-	Horne et al., 1983
Amphipod, <i>Gammarus minus</i>	A	E	fluoranthene (206-44-0)	5.08	S	U	32	0.16	0.16	10.1	13.6	-	Horne and Oblad, 1983
Amphipod, <i>Gammarus pseudolimnaeus</i>	X	E	fluorene (86-73-7)	4.21	S	U	600	3.61	3.61	34.2	-	-	Finger et al., 1985
Amphipod, <i>Gammarus pseudolimnaeus</i>	X	E	phenanthrene (85-01-8)	4.57	FT	M	126	0.707	0.707	14.8	-	-	Call et al., 1986
Amphipod, <i>Gammarus pseudolimnaeus</i>	A	E	fluoranthene (206-44-0)	5.08	FT	M	43	0.213	0.213	13.5	19.0	16.1	Spehar et al., 1999
Amphipod, <i>Hyalella azteca</i>	J	E	fluoranthene (206-44-0)	5.08	FT	M	44	0.218	0.218	13.9	13.9	13.9	Spehar et al., 1999
Dragonfly, <i>Ophiogomphus</i> sp.	N	E	fluoranthene (206-44-0)	5.08	FT	M	>178	>0.880	>0.880	>56	>56	>56	Spehar et al., 1999
Stonefly, <i>Peltoperla maria</i>	X	E	acenaphthene (83-32-9)	4.01	S	U	240	1.6	1.6	9.6	-	-	Horne et al., 1983

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^A	HABITAT ^a	PAH TESTED (CAS #)	LOG K _{ow} ^c	METHOD ^b	CONCENTRATION ^b	LC50/EC50 ^b (μg/L)	LC50/EC50 ^b (μmol/L)	PAH SPECIFIC SMAV ⁱⁱ (μmol/L)	K _{ow} NORMALIZED PAH SPECIFIC SMAV ⁱ (μmol/g _{oc})	SPECIES SMAV ^j (μmol/g _{oc})	GMAV ^k (μmol/g _{oc})	REFERENCES
Stonefly, <i>Peltopera maria</i>	X	E	fluoranthene (206-44-0)	5.08	S	U	135	0.667	0.667	42.5	20.2	20.2	Horne and Oblad, 1983
Midge, <i>Chironomus tentans</i>	L	I	naphthalene (91-20-3)	3.36	S	M	2810	21.9	21.9	32.5	-	-	Millemann et al., 1984
Midge, <i>Chironomus tentans</i>	L	I	phenanthrene (85-01-8)	4.57	S	M	490	2.75	2.75	57.0	-	-	Millemann et al., 1984
Midge, <i>Chironomus tentans</i>	L	I	fluoranthene (206-44-0)	5.08	S	M	>250	>1.24	>1.24	>79 ^h	43.0	-	Suedel and Rodgers, 1996
Midge, <i>Chironomus riparius</i>	L	I	fluorene (86-73-7)	4.21	S	U	>1900 (2350)	>11.42	>11.42	>108	>108	>68.2	Finger et al., 1985
Midge, <i>Paratanytarsus sp.</i>	X	E	acenaphthene (83-32-9)	4.01	S	M	2000	13.0	-	-	-	-	Northwestern Aquatic Science Inc., 1982
Midge, <i>Paratanytarsus sp.</i>	X	E	acenaphthene (83-32-9)	4.01	S	M	2090	13.6	13.3	82	82	82	Northwestern Aquatic Science Inc., 1982
Midge <i>Tanytarsus dissimilis</i>	L	I	naphthalene (91-20-3)	3.36	S	U	20700	162	-	-	-	-	Darville and Wilhm, 1984
Midge <i>Tanytarsus dissimilis</i>	L	I	naphthalene (91-20-3)	3.36	S	U	12600	98.31	126	187	187	187	Darville and Wilhm, 1984
Coho salmon <i>Oncorhynchus kisutch</i>	E	I	naphthalene (91-20-3)	3.36	R	M	>11800	>92.1	-	-	-	-	Korn and Rice, 1981
Coho salmon <i>Oncorhynchus kisutch</i>	F	W	naphthalene (91-20-3)	3.36	R	M	5600	43.7	43.7	65.0	65.0	-	Korn and Rice, 1981
Rainbow trout <i>Oncorhynchus mykiss</i>	pre SU	I	naphthalene (91-20-3)	3.36	S	U	1800	14.0	-	-	-	-	Edsall, C.C., 1991
Rainbow trout <i>Oncorhynchus mykiss</i>	pre SU	I	naphthalene (91-20-3)	3.36	S	U	6100	47.6	-	-	-	-	Edsall, C.C., 1991

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									SMAV ^H (μmol/L)	PAH SPECIFIC SMAV ^I (μmol/g _{cc})	SMAV ^J (μmol/g _{cc})		
Rainbow trout <i>Oncorhynchus mykiss</i>	pre SU	I	naphthalene (91-20-3)	3.36	S	U	2600	20.3	-	-	-	-	Edsall, C.C., 1991
Rainbow trout <i>O. corhynchus mykiss</i>	pre SU	I	naphthalene (91-20-3)	3.36	S	U	4400	34.3	-	-	-	-	Edsall, C.C., 1991
Rainbow trout <i>Oncorhynchus mykiss</i>	pre SU	I	naphthalene (91-20-3)	3.36	S	U	5500	42.9	-	-	-	-	Edsall, C.C., 1991
Rainbow trout <i>Oncorhynchus mykiss</i>	J	W	naphthalene (91-20-3)	3.36	FT	M	1600	12.5	-	-	-	-	DeGraeve et al., 1982
Rainbow trout <i>Oncorhynchus mykiss</i>	X	W	naphthalene (91-20-3)	3.36	FT	M	2300	17.9	15.0	22.2	-	-	DeGraeve et al., 1980
Rainbow trout <i>Oncorhynchus mykiss</i>	J	W	acenaphthene (83-32-9)	4.01	FT	M	670	4.34	4.34	26.9	-	-	Holcombe et al., 1983
Rainbow trout <i>Oncorhynchus mykiss</i>	J	W	fluorene (86-73-7)	4.21	S	U	820	4.93	4.93	46.7	-	-	Finger et al., 1985
Rainbow trout <i>Oncorhynchus mykiss</i>	pre SU	I	1,3-dimethyl naphthalene (575-41-7)	4.37	S	U	1700	10.9	14.0	188 ^L	-	-	Edsall, C.C., 1991
Rainbow trout <i>Oncorhynchus mykiss</i>	L	W	phenanthrene (85-01-8)	4.57	S	U	> 1100 (3200)	> 6.2	-	-	-	-	Edsall, C.C., 1991
Rainbow trout <i>Oncorhynchus mykiss</i>	J	W	phenanthrene (85-01-8)	4.57	FT	M	375	2.10	2.10	43.9	-	-	Call et al., 1986
Rainbow trout <i>Oncorhynchus mykiss</i>	X	W	fluoranthene (206-44-0)	5.08	S	M	187	0.925	-	-	-	-	Horne and Oblad, 1983
Rainbow trout <i>Oncorhynchus mykiss</i>	J	W	fluoranthene (206-44-0)	5.08	FT	M	26.0	0.129	0.129	8.19	25.1	40.4	Spehar et al., 1999
Brown trout, <i>Salmo trutta</i>	J	W	acenaphthene (83-32-9)	4.01	FT	M	580	3.76	3.76	23.3	23.3	23.3	Holcombe et al., 1983

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									SMAV ^H (μmol/L)	PAH SPECIFIC SMAV ^I (μmol/g _{oc})	SMAV ^I (μmol/g _{oc})	(μmol/g _{oc})	
Fathead minnow, <i>Pimephales promelas</i>	J	W	naphthalene (91-20-3)	3.36	S	M	1990	15.5	-	-	-	-	Millermann et al., 1984
Fathead minnow, <i>Pimephales promelas</i>	J	W	naphthalene (91-20-3)	3.36	FT	M	7900	61.6	-	-	-	-	DeGraeve et al., 1982
Fathead minnow, <i>Pimephales promelas</i>	X	W	naphthalene (91-20-3)	3.36	FT	M	4900	38.2	-	-	-	-	DeGraeve et al., 1980
Fathead minnow, <i>Pimephales promelas</i>	J	W	naphthalene (91-20-3)	3.36	FT	M	6140	47.9	-	-	-	-	Geiger et al., 1985
Fathead minnow, <i>Pimephales promelas</i>	J	W	naphthalene (91-20-3)	3.36	FT	M	8900	69.4	-	-	-	-	DeGraeve et al., 1980
Fathead minnow, <i>Pimephales promelas</i>	J	W	naphthalene (91-20-3)	3.36	FT	M	6080	47.4	51.8	76.8	-	-	Holcombe et al., 1984
Fathead minnow, <i>Pimephales promelas</i>	J	W	1-methyl naphthalene (90-12-0)	3.84	S	U	9000	63.4	63.4	268	-	-	Mattson et al., 1976
Fathead minnow, <i>Pimephales promelas</i>	J	W	acenaphthene (83-32-9)	4.01	S	M	3100	20	-	-	-	-	Marine Bioassay Lab., 1981
Fathead minnow, <i>Pimephales promelas</i>	J	W	acenaphthene (83-32-9)	4.01	S	M	1500	9.7	-	-	-	-	EG&G Bionomics, 1982
Fathead minnow, <i>Pimephales promelas</i>	A	W	acenaphthene (83-32-9)	4.01	R	U	3700	24	-	-	-	-	Academy of Natural Sci., 1981
Fathead minnow, <i>Pimephales promelas</i>	J	W	acenaphthene (83-32-9)	4.01	FT	M	1730	11.2	-	-	-	-	Geiger et al., 1985
Fathead minnow, <i>Pimephales promelas</i>	J	W	acenaphthene (83-32-9)	4.01	FT	M	608	3.94	-	-	-	-	Cairns and Nebeker, 1982
Fathead minnow,	J	W	acenaphthene	4.01	FT	M	>1400	>9.1	-	-	-	-	EG&G Bionomics, 1982

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<i>Pimephales promelas</i>			(83-32-9)										
Fathead minnow, <i>Pimephales promelas</i>	J	W	acenaphthene (83-32-9)	4.01	FT	M	1600	10	7.71	48.0	-	-	Holcombe et al., 1983
Fathead minnow, <i>Pimephales promelas</i>	X	W	fluorene (86-73-7)	4.21	S	U	> 1900 (100000)	> 11.4	> 11.4	> 108 ^L	-	-	Finger et al., 1985
Fathead minnow, <i>Pimephales promelas</i>	J	W	phenanthrene (85-01-8)	4.57	S	M	> 1100 (> 1150)	> 6.17	> 6.17	> 129 ^L	-	-	U.S. EPA, 1978
Fathead minnow, <i>Pimephales promelas</i>	J	W	fluoranthene (206-44-0)	5.08	S	M	95	0.470	-	-	-	-	Horne and Oblad, 1983
Fathead minnow, <i>Pimephales promelas</i>	J	W	fluoranthene (206-44-0)	5.08	S	M	7.71	0.0381	-	-	-	-	Gendusa, 1990
Fathead minnow, <i>Pimephales promelas</i>	A	W	fluoranthene (206-44-0)	5.08	FT	U	> 260 (> 1000)	> 1.29	-	-	-	-	Birge et al., 1982
Fathead minnow, <i>Pimephales promelas</i>	J	W	fluoranthene (206-44-0)	5.08	FT	M	69	0.34	0.34	22.0	68.3	68.3	Spehar et al., 1999
Channel catfish, <i>Ictalurus punctatus</i>	J	E	acenaphthene (83-32-9)	4.01	FT	M	1720	11.2	11.2	69.0	-	-	Holcombe et al., 1983
Channel catfish, <i>Ictalurus punctatus</i>	J	E	fluoranthene (206-44-0)	5.08	S	M	37.40	0.185	0.185	12.0	28.8	28.8	Gendusa, 1990
Bluegill, <i>Lepomis macrochirus</i>	J	W	acenaphthene (83-32-9)	4.01	S	U	1700	11.0	11.0	68	-	-	Buccafusco et al., 1981
Bluegill, <i>Lepomis macrochirus</i>	X	W	fluorene (86-73-7)	4.21	S	U	910	5.47	5.47	51.8	-	-	Finger et al., 1985
Bluegill, <i>Lepomis macrochirus</i>	J	W	phenanthrene (85-01-8)	4.57	FT	M	234	1.31	1.31	27.4	-	-	Call et al., 1986

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Bluegill, <i>Lepomis macrochirus</i>	J	W	fluoranthene (206-44-0)	5.08	S	U	>260 (4000)	>1.3	-	-	-	-	Buccafusco et al., 1981; EPA, 1978
Bluegill, <i>Lepomis macrochirus</i>	J	W	fluoranthene (206-44-0)	5.08	FT	M	44	0.218	0.218	13.9	34.0	34.0	Spehar et al., 1999
South african clawed frog <i>Xenopus laevis</i>	L	W	naphthalene (91-20-3)	3.36	FT	M	2100	16.38	-	-	-	-	Edmisten and Bantle, 1982
South african clawed frog <i>Xenopus laevis</i>	L	W	naphthalene (91-20-3)	3.36	FT	M	2100	16.38	16.38	24.3	24.3	24.3	Edmisten and Bantle, 1982
<u>SALTWATER</u>													
Annelid worm, <i>Neanthes arenaceodentata</i>	J	I	naphthalene (91-20-3)	3.36	S	U	3800	29.6	29.6	44.0	-	-	Rossi and Neff, 1978
Annelid worm, <i>Neanthes arenaceodentata</i>	X	I	acenaphthene (83-32-9)	4.01	S	U	3600	23.3	-	-	-	-	Horne et al., 1983
Annelid worm, <i>Neanthes arenaceodentata</i>	J	I	acenaphthene (83-32-9)	4.01	R	U	>3800 (16440)	>24.6	23.3	144	-	-	Thursby et al., 1989a
Annelid worm, <i>Neanthes arenaceodentata</i>	A	I	phenanthrene (85-01-8)	4.57	S	U	600	3.37	3.37	70.0	-	-	Rossi and Neff, 1978
Annelid worm, <i>Neanthes arenaceodentata</i>	J	I	fluoranthene (206-44-0)	5.08	S	U	>260 (500)	>1.29	-	-	-	-	Rossi and Neff, 1978
Annelid worm, <i>Neanthes arenaceodentata</i>	J	I	fluoranthene (206-44-0)	5.08	S	U	>260 (20000)	>1.29	>1.29	>82 ^L	76.3	76.3	Spehar et al., 1999
Archiannelid, <i>Dinophilus gyrociliatus</i>	J	I	phenanthrene (85-01-8)	4.57	R	U	185.40	1.04	1.04	21.7	21.7	21.7	Battelle Ocean Sciences, 1987
Mud snail, <i>Nassarius obsoletus</i>	A	I,E	phenanthrene (85-01-8)	4.57	R	M	>245	>1.37	>1.37	>28.7	>28.7	>28.7	Battelle Ocean Sciences, 1987

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Blue mussel, <i>Mytilus edulis</i>	A	E,W	phenanthrene (85-01-8)	4.57	R	M	>245	>1.37	>1.37	>28.7	>28.7	>28.7	Battelle Ocean Sciences, 1987
Pacific oyster, <i>Crassostrea gigas</i>	E/L	W	naphthalene (91-20-3)	3.36	S	U	>31000 (199000)	>242	>242	>359	>359	>359	U.S. EPA, 1980
Coot clam, <i>Mulinia lateralis</i>	J	E	pyrene (129-00-0)	4.92	FT	M	>132 (>240)	>0.653	>0.653	>29.2	-	-	Champlin and Poucher, 1992c
Coot clam, <i>Mulinia lateralis</i>	J	E	fluoranthene (206-44-0)	5.08	S	U	>260 (10710)	>1.29	>1.29	>82.0	>48.9	>48.9	Spehar et al., 1999
Soft-shell clam, <i>Mya arenaria</i>	A	I	phenanthrene (85-01-8)	4.57	R	M	>245	>1.37	>1.37	>28.7	>28.7	>28.7	Battelle Ocean Sciences, 1987
Calanoid copepod <i>Eurytemora affinis</i>	A	X	naphthalene (91-20-3)	3.36	S	U	3798	22.6	22.6	33.5	-	-	Ott, et al., 1978
Calanoid copepod <i>Eurytemora affinis</i>	A	X	2-methyl naphthalene (91-57-6)	3.86	S	U	1499	7.74	7.74	34.2	-	-	Ott, et al., 1978
Calanoid copepod <i>Eurytemora affinis</i>	A	X	2,6-dimethyl naphthalene (581-42-0)	4.37	S	M	852	3.9	3.9	52.0	-	-	Ott, et al., 1978
Calanoid copepod <i>Eurytemora affinis</i>	A	X	2,3,5-trimethyl naphthalene (2245-38-7)	4.86	S	M	316	1.3	1.3	50.0	41.5	41.5	Ott, et al., 1978
Mysid, <i>Americamysis bahia</i>	J	E	acenaphthene (83-32-9)	4.01	S	U	970	6.29	-	-	-	-	U.S. EPA, 1978; Ward et al., 1981
Mysid, <i>Americamysis bahia</i>	J	E	acenaphthene (83-32-9)	4.01	S	M	160	1.04	-	-	-	-	EG&G Bionomics, 1982
Mysid, <i>Americamysis bahia</i>	J	E	acenaphthene (83-32-9)	4.01	R	U	1190	7.72	-	-	-	-	Thursby et al., 1989a

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Mysid, <i>Americamysis bahia</i>	J	E	acenaphthene (83-32-9)	4.01	FT	M	460	2.98	-	-	-	-	Thursby et al., 1989b
Mysid, <i>Americamysis bahia</i>	J	E	acenaphthene (83-32-9)	4.01	FT	M	190	1.23	-	-	-	-	EG&G Bionomics, 1982
Mysid, <i>Americamysis bahia</i>	J	E	acenaphthene (83-32-9)	4.01	FT	M	466.1	3.02	-	-	-	-	Horne et al., 1983; Thursby, 1991a
Mysid, <i>Americamysis bahia</i>	J	E	acenaphthene (83-32-9)	4.01	FT	M	271.9	1.76	2.10	13.0	-	-	Horne et al., 1983; Thursby, 1991a
Mysid, <i>Americamysis bahia</i>	J	E	phenanthrene (85-01-8)	4.57	FT	M	27.1	0.152	-	-	-	-	Kuhn and Lussier, 1987
Mysid, <i>Americamysis bahia</i>	J	E	phenanthrene (85-01-8)	4.57	FT	M	17.7	0.099	0.123	2.60	-	-	Battelle Ocean Sciences, 1987
Mysid, <i>Americamysis bahia</i>	J	E	pyrene (129-00-0)	4.92	FT	M	28.28	0.140	0.140	6.30	-	-	Champlin and Poucher, 1992c
Mysid, <i>Americamysis bahia</i>	J	E	fluoranthene (206-44-0)	5.08	S	U	31	0.153	-	-	-	-	Spehar et al., 1999
Mysid, <i>Americamysis bahia</i>	J	E	fluoranthene (206-44-0)	5.08	S	U	40	0.198	-	-	-	-	U.S. EPA, 1978
Mysid, <i>Americamysis bahia</i>	J	E	fluoranthene (206-44-0)	5.08	FT	M	30.53	0.151	-	-	-	-	Champlin and Poucher, 1992b; Spehar et al., 1999
Mysid, <i>Americamysis bahia</i>	J	E	fluoranthene (206-44-0)	5.08	FT	M	87	0.430	0.255	16.2	7.66	7.66	EG&G Bionomics, 1978
Mysid, <i>Neomysis americana</i>	X	E	naphthalene (91-20-3)	3.36	S	M	1250	9.75	-	-	-	-	Hargreaves et al., 1982
Mysid, <i>Neomysis americana</i>	X	E	naphthalene (91-20-3)	3.36	S	M	1420	11.1	10.4	15.4	15.4	15.4	Hargreaves et al., 1982

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Isopod <i>Excirrolana vancouverensis</i>	J	I,E	fluoranthene (206-44-0)	5.08	R	M	> 70	> 0.346	> 0.346	> 22.1	> 22.1	> 22.1	Boese et al., 1997
Amphipod, <i>Ampelisca abdita</i>	J	I	acenaphthene (83-32-9)	4.01	R	U	1125	7.30	7.30	45.1	-	-	Thursby et al., 1989a
Amphipod, <i>Ampelisca abdita</i>	J	I	fluoranthene (206-44-0)	5.08	S	U	67	0.33	0.33	21.1	30.8	30.8	Spehar et al., 1999
Amphipod, <i>Leptocheirus plumulosus</i>	A	E,I	acenaphthene (83-32-9)	4.01	FT	M	589.4	3.82	3.82	23.6	-	-	Swartz, 1991a
Amphipod, <i>Leptocheirus plumulosus</i>	A	E,I	phenanthrene (85-01-8)	4.57	FT	M	198.4	1.11	1.11	23.2	-	-	Swartz, 1991a
Amphipod, <i>Leptocheirus plumulosus</i>	J	E,I	pyrene (129-00-0)	4.92	FT	M	66.49	0.329	0.329	14.7	-	-	Champlin and Poucher, 1992
Amphipod, <i>Leptocheirus plumulosus</i>	X	E,I	fluoranthene (206-44-0)	5.08	R	M	51	0.252	0.252	16.1	19.0	19.0	Boese et al., 1997
Amphipod, <i>Rhepoxynius abronius</i>	J	I	fluoranthene (206-44-0)	5.08	R	M	63	0.311	0.311	19.9	19.9	19.9	Boese et al., 1997
Amphipod, <i>Eohaustorius estuarius</i>	J	I	fluoranthene (206-44-0)	5.08	R	M	> 70	> 0.346	> 0.346	> 22.1	> 22.1	> 22.1	Boese et al., 1997
Amphipod, <i>Grandidierella japonica</i>	J	I	fluoranthene (206-44-0)	5.08	R	M	27	0.133	0.133	8.5	8.5	8.5	Boese et al., 1997
Amphipod, <i>Corophium insidiosum</i>	J	I	fluoranthene (206-44-0)	5.08	R	M	54	0.267	0.267	17.0	17.0	17.0	Boese et al., 1997
Amphipod, <i>Emerita analoga</i>	J	I,E	fluoranthene (206-44-0)	5.08	R	M	74	0.366	0.366	23.3	23.3	23.3	Boese et al., 1997
Kelp shrimp	X	W	naphthalene	3.36	FT	M	1390	10.8	10.8	16.1	16.1	16.1	Rice and Thomas, 1989

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^a	HABITAT ^b	PAH TESTED (CAS #)	LOG K _{ow} ^c	METHOD ^d	CONCENTRATION ^e	LC50/EC50 ^f (μg/L)	LC50/EC50 ^g (μmol/L)	PAH SPECIFIC SMAV ^h (μmol/L)	K _{ow} NORMALIZED PAH SPECIFIC SMAV ⁱ (μmol/g _{oc})	SPECIES SMAV ^j (μmol/g _{oc})	GMAV ^k (μmol/g _{oc})	REFERENCES
<i>Eualis suckleyi</i>			(91-20-3)										
Grass shrimp, <i>Palaemonetes pugio</i>	X	E, W	naphthalene (91-20-3)	3.36	S	M	2350	18.3	18.3	27.2	-	-	Tatem et al., 1978
Grass shrimp, <i>Palaemonetes pugio</i>	X	E, W	acenaphthene (83-32-9)	4.01	S	U	676.8	4.39	-	-	-	-	Horne et al., 1983; Thursby, 1991b
Grass shrimp, <i>Palaemonetes pugio</i>	L	E, W	acenaphthene (83-32-9)	4.01	R	U	1697	11.0	6.95	43.0	-	-	Thursby et al., 1989a
Grass shrimp, <i>Palaemonetes pugio</i>	A	E, W	phenanthrene (85-01-8)	4.57	R	U	200.8	1.127	-	-	-	-	Battelle Ocean Sciences, 1987
Grass shrimp, <i>Palaemonetes pugio</i>	A	E, W	phenanthrene (85-01-8)	4.57	FT	M	145.4	0.816	0.816	17.0	-	-	Battelle Ocean Sciences, 1987
Grass shrimp, <i>Palaemonetes pugio</i>	J	E, W	fluoranthene (206-44-0)	5.08	S	U	142	0.702	0.702	44.7	30.7	30.7	Spehar et al., 1999
Sand shrimp, <i>Crangon septemspinosus</i>	X	E	acenaphthene (83-32-9)	4.01	S	U	245	1.59	1.59	4.80	9.80	9.80	Horne et al., 1983; Thursby, 1991b
American Lobster, <i>Homarus americanus</i>	L	-	fluoranthene (206-44-0)	5.08	R	U	>260 (317)	1.29	1.29	81.9	81.9	81.9	Spehar et al., 1999
Hermit crab, <i>Pagurus longicarpus</i>	A	E	phenanthrene (85-01-8)	4.57	FT	M	163.7	0.918	0.918	19.2	19.2	19.2	Battelle Ocean Sciences, 1987
Slipper limpet, <i>Crepidula fornicata</i>	L	W	acenaphthene (83-32-9)	4.01	R	U	3436	22.3	22.3	138	138	138	Thursby et al., 1989a
Sea urchin, <i>Arbacia punctulata</i>	E	W	acenaphthene (83-32-9)	4.01	S	U	>3800 (8163)	>24.6	>24.6	>152	-	-	Thursby et al., 1989a
Sea urchin, <i>Arbacia punctulata</i>	E	W	fluoranthene (206-44-0)	5.08	S	U	>260 (20000)	>1.3	>1.3	>82	>117	>117	Spehar et al., 1999

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^A	HABITAT ^B	PAH TESTED (CAS #)	LOG K _{ow} ^C	METHOD ^D	CONCENTRATION ^E	LC50/EC50 ^F (μg/L)	LC50/EC50 ^F (μmol/L)	PAH SPECIFIC SMAV ^H (μmol/L)	K _{ow} NORMALIZED PAH SPECIFIC SMAV ^I (μmol/g _{oc})	SPECIES SMAV ^J (μmol/g _{oc})	GMAV ^K (μmol/g _{oc})	REFERENCES
Pink salmon, <i>Oncorhynchus gorbuscha</i>	Fry	W	naphthalene (91-20-3)	3.36	FT	M	960	7.49	-	-	-	-	Rice and Thomas, 1989
Pink salmon, <i>Oncorhynchus gorbuscha</i>	Fry	W	naphthalene (91-20-3)	3.36	FT	M	900	7.02	-	-	-	-	Rice and Thomas, 1989
Pink salmon, <i>Oncorhynchus gorbuscha</i>	Fry	W	naphthalene (91-20-3)	3.36	FT	M	990	7.72	-	-	-	-	Rice and Thomas, 1989
Pink salmon, <i>Oncorhynchus gorbuscha</i>	Fry	W	naphthalene (91-20-3)	3.36	FT	M	1010	7.88	-	-	-	-	Rice and Thomas, 1989
Pink salmon, <i>Oncorhynchus gorbuscha</i>	Fry	W	naphthalene (91-20-3)	3.36	FT	M	890	6.94	7.40	11.0	11.0	11.0	Rice and Thomas, 1989
Sheepshead minnow, <i>Cyprinodon variegatus</i>	J	E,W	acenaphthene (83-32-9)	4.01	S	U	2200	14.3	-	-	-	-	Heitmuller et al., 1981
Sheepshead minnow, <i>Cyprinodon variegatus</i>	J	E,W	acenaphthene (83-32-9)	4.01	R	U	>3800 (50000)	>25	-	-	-	-	Thursby et al., 1989a
Sheepshead minnow, <i>Cyprinodon variegatus</i>	A	E,W	acenaphthene (83-32-9)	4.01	FT	M	3100	20.1	20.1	124	-	-	Ward et al., 1981
Sheepshead minnow, <i>Cyprinodon variegatus</i>	J	E,W	phenanthrene (85-01-8)	4.57	R	U	>245	>1.37	-	-	-	-	Battelle Ocean Sciences, 1987
Sheepshead minnow, <i>Cyprinodon variegatus</i>	J	E,W	phenanthrene (85-01-8)	4.57	FT	M	429.4	2.41	2.41	50.0	-	-	Battelle Ocean Sciences, 1987
Sheepshead minnow, <i>Cyprinodon variegatus</i>	J	E,W	pyrene (129-00-0)	4.92	FT	M	>132 (>640)	>0.653	>0.653	>29.2	-	-	Champlin and Poucher, 1992b
Sheepshead minnow, <i>Cyprinodon variegatus</i>	J	E,W	fluoranthene (206-44-0)	5.08	S	U	>260 (>20000)	>1.29	-	-	-	-	Champlin and Poucher, 1992a; Spehar et al., 1999
Sheepshead minnow, <i>Cyprinodon variegatus</i>	J	E,W	fluoranthene (206-44-0)	5.08	S	U	>260 (>560000)	>1.29	>1.29	>82 ^L	78.7	78.7	Heitmuller et al., 1981; U.S EPA, 1978

COMMON/SCIENTIFIC NAME	LIFE-STAGE ^A	HABITAT ^B	PAH TESTED (CAS #)	LOG K _{ow} ^C	METHOD ^D	CONCENTRATION ^E	LC50/EC50 ^F (μg/L)	LC50/EC50 ^F (μmol/L)	PAH SPECIFIC SMAV ^H (μmol/L)	K _{ow} NORMALIZED PAH SPECIFIC SMAV ^I (μmol/g _{oc})	SPECIES SMAV ^J (μmol/g _{oc})	GMAV ^K (μmol/g _{oc})	REFERENCES
Inland silverside, <i>Menidia beryllina</i>	X	W	acenaphthene (83-32-9)	4.01	S	U	2300	14.9	-	-	-	-	Horne et al., 1983
Inland silverside, <i>Menidia beryllina</i>	J	W	acenaphthene (83-32-9)	4.01	R	U	> 3800 (5564)	> 24.6	> 19.2	> 150	-	-	Thursby et al., 1989a
Inland silverside, <i>Menidia beryllina</i>	J	W	pyrene (192-00-0)	4.92	FT	M	> 132 (> 188.17)	> 0.653	> 0.653	> 29.2	-	-	Champlin and Poucher, 1992
Inland silverside, <i>Menidia beryllina</i>	J	W	fluoranthene (206-44-0)	5.08	S	U	> 260 (> 616)	> 1.29	> 1.29	> 82.0	> 65.8	-	Spehar et al., 1999
Atlantic silverside, <i>Menidia menidia</i>	A	W	phenanthrene (85-01-8)	4.57	FT	M	108	0.606	0.606	12.6	12.6	28.8	Battelle Ocean Sciences, 1987
Winter flounder,	J	-	fluoranthene (206-44-0)	5.08	S	M	> 188	> 0.929	> 0.929	> 59.2	> 59.2	> 59.2	Spehar et al., 1999

^ALife-stage: A = adult, J = juvenile, L = larvae, E = embryo, U = life-stage and habitat unknown, X = life-stage unknown but habitat known.

^BHabitat: I = infauna, E = epibenthic, W = water column.

^Clog K_{ow}: Predicted using SPARC (Karickhoff et al, 1991).

^DMethod: S = static, R = renewal, FT = flow-through.

^EConcentration: U = unmeasured (nominal), M = chemical measured.

^FAcute Values: 96 hour LC50 or EC50, except for *Daphnia* and *Tanytarsus* which are 48 hours duration.

^GBolded acute values are the water solubilities of the PAH (Mackay et al., 1992). For these tests the acute values exceeded solubility. Therefore, solubilities are used instead of the acute value for further calculations.

^HPAH-specific SMAV: Geometric mean of the acute values by PAH and species.

^IPAH-specific SMAVs at a log K_{ow} = 1.0; calculated as antilog (log₁₀LC50 + 0.945log₁₀K_{ow})/1000 (see Equation 2-33).

^JSpecies SMAV: Geometric mean of K_{ow}-normalized SMAVs for a species across PAHs.

^KGMAV: Geometric mean of SMAVs for all species within a genus.

^LNot used in calculations.

APPENDIX D. Comparison of PAH-specific equilibrium partitioning sediment guidelines (ESGs) derived from narcosis theory and the median response concentration of benthic species for individual PAHs in spiked-sediment toxicity tests.

Common Name, <i>Scientific Name</i>	Chemical	Response	Median Response Conc. ^A ($\mu\text{g/goc}$)	$C_{OC,PAH,FCVI}$ ($\mu\text{g/goc}$)	Test- Specific $\text{ESG}_{\text{FCVI}}^{\text{B}}$ (Unitless)	PAH- Specific SMAV^{C}	GMAV^{D}	References ^E
Oligochaete, <i>Lumbriculus variegatus</i>	pyrene	7 d LC50	> 9090 (61100)	694	> 13.1	-	-	Kukkonen and Landrum, 1994
Ol gochaete, <i>Lumbriculus variegatus</i>	pyrene	7 d EC50-SA	> 9090 (51400)	694	> 13.1	-	-	Kukkonen and Landrum, 1994
Oligochaete, <i>Limnodrilus hoffmeisteri</i>	phenanthrene	10 d LC50	> 34300 (42500)	593	> 57.8	> 57.8	> 57.8	Lotufo and Fleeger, 1996
Oligochaete, <i>Limnodrilus hoffmeisteri</i>	phenanthrene	28 d EC25-R	5790	593	9.80	-	-	Lotufo and Fleeger, 1996
Oligochaete, <i>Limnodrilus hoffmeisteri</i>	pyrene	28 d EC25-R	8440	694	12.2	-	-	Lotufo and Fleeger, 1996
Cladoceran, <i>Daphnia magna</i>	fluoranthene	10 d LC50	2380	704	-	-	-	Suedel et al., 1993
Cladoceran, <i>Daphnia magna</i>	fluoranthene	10 d LC50	955	704	-	-	-	Suedel et al., 1993
Cladoceran, <i>Daphnia magna</i>	fluoranthene	10 d LC50	3260	704	-	-	-	Suedel et al., 1993
Amphipod, <i>Hyalella azteca</i>	fluoranthene	10 d LC50	> 23900 (37649)	704	-	-	-	Driscoll et al., 1997a
Amphipod, <i>Hyalella azteca</i>	fluoranthene	10 d LC50	1250	704	-	-	-	Suedel et al., 1993
Amphipod, <i>Hyalella azteca</i>	fluoranthene	10 d LC50	1480	704	-	-	-	Suedel et al., 1993
Amphipod, <i>Hyalella azteca</i>	fluoranthene	10 d LC50	500	704	-	-	-	Suedel et al., 1993
Amphipod, <i>Hyalella azteca</i>	fluoranthene	10 d LC50	22000	704	31.3	-	-	Harkey et al., 1997

Common Name, Scientific Name	Chemical	Response	Median Response Conc. ^A (µg/goc)	C _{OC,PAH,FCVI} (µg/goc)	Test- Specific ESGU _{FCVI} ^B (Unitless)	PAH- Specific SMAV ^C	GMAV ^D	References ^E
Amphipod, <i>Hyaella azteca</i>	fluoranthene	10 d LC50	5130	704	7.29	15.1	15.1	DeWitt et al., 1989
Amphipod, <i>Corophium spinicorne</i>	fluoranthene	10 d LC50	2830	704	4.02	-	-	Swartz et al., 1990
Amphipod, <i>Corophium spinicorne</i>	fluoranthene	10 d LC50	4390	704	6.23	5.01	5.01	Swartz et al., 1990
Amphipod, <i>Leptocheirus plumulosus</i>	acenaphthene	10 d LC50	10900	489	22.3	-	-	Swartz et al., 1991a
Amphipod, <i>Leptocheirus plumulosus</i>	acenaphthene	10 d LC50	23500	489	48.1	-	-	Swartz et al., 1991a
Amphipod, <i>Leptocheirus plumulosus</i>	acenaphthene	10 d LC50	8450	489	17.3	26.4	-	Swartz et al., 1991a
Amphipod, <i>Leptocheirus plumulosus</i>	phenanthrene	10 d LC50	6870	593	11.59	-	-	Swartz et al., 1991a
Amphipod, <i>Leptocheirus plumulosus</i>	phenanthrene	10 d LC50	8080	593	13.63	-	-	Swartz et al., 1991a
Amphipod, <i>Leptocheirus plumulosus</i>	phenanthrene	10 d LC50	8180	593	13.8	13.0	18.5	Swartz et al., 1991a
Amphipod, <i>Rhepoxynius abronius</i>	acenaphthene	10 d LC50	2310	489	4.72	-	-	Swartz et al., 1997
Amphipod, <i>Rhepoxynius abronius</i>	acenaphthene	10 d LC50	2110	489	4.31	4.51	-	Swartz et al., 1997
Amphipod, <i>Rhepoxynius abronius</i>	phenanthrene	10 d LC50	3080	593	5.19	-	-	Swartz et al., 1997
Amphipod, <i>Rhepoxynius abronius</i>	phenanthrene	10 d LC50	2220	593	3.74	4.41	-	Swartz et al., 1997
Amphipod, <i>Rhepoxynius abronius</i>	pyrene	10 d LC50	1220	694	1.76	-	-	Swartz et al., 1997

Common Name, Scientific Name	Chemical	Response	Median Response Conc. ^A (µg/goc)	C _{OC,PAH,FCVI} (µg/goc)	Test- Specific ESGU _{PCVI} ^B (Unitless)	PAH- Specific SMAV ^C	GMAV ^D	References ^E
Amphipod, <i>Rhepoxynius abronius</i>	pyrene	10 d LC50	2810	694	4.05	2.67	-	Swartz et al., 1997
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	> 4360	704	> 6.19	-	-	DeWitt et al., 1992
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	4410	704	6.26	-	-	DeWitt et al., 1992
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	3080	704	4.38	-	-	DeWitt et al., 1992
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	2230	704	3.17	-	-	Swartz et al., 1990
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	3150	704	4.50	-	-	DeWitt et al., 1992
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	1890	704	2.68	-	-	Swartz et al., 1990
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	2790	704	3.96	-	-	De Witt et al., 1992
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	2320	704	3.30	-	-	Swartz et al., 1997
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	1700	704	2.41	-	-	DeWitt et al., 1989
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	1030	704	1.47	-	-	Swartz et al., 1988
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	2100	704	2.98	-	-	Swartz et al., 1990
Amphipod, <i>Rhepoxynius abronius</i>	fluoranthene	10 d LC50	3310	704	4.70	3.56	3.67	Swartz et al., 1997
Amphipod, <i>Eohaustorius estuarius</i>	acenaphthene	10 d LC50	1630	489	3.33	-	-	Swartz et al., 1991a
Amphipod,	acenaphthene	10 d LC50	4180	489	8.55	-	-	Swartz et al., 1991a

Common Name, <i>Scientific Name</i>	Chemical	Response	Median Response Conc. ^A ($\mu\text{g/goc}$)	$C_{OC,PAH,FCVI}$ ($\mu\text{g/goc}$)	Test- Specific ESGU _{FCVI} ^B (Unitless)	PAH- Specific SMAV ^C	GMAV ^D	References ^E
<i>Eohaustorius estuarius</i>								
Amphipod, <i>Eohaustorius estuarius</i>	acenaphthene	10 d LC50	1920	489	3.93	4.82	-	Swartz et al., 1991a
Amphipod, <i>Eohaustorius estuarius</i>	phenanthrene	10 d LC50	4210	593	7.10	-	-	Swartz et al., 1991a
Amphipod, <i>Eohaustorius estuarius</i>	phenanthrene	10 d LC50	3760	593	6.34	-	-	Swartz et al., 1991a
Amphipod, <i>Eohaustorius estuarius</i>	phenanthrene	10 d LC50	4060	593	6.85	6.75	-	Swartz et al., 1991a
Amphipod, <i>Eohaustorius estuarius</i>	fluoranthene	10 d LC50	3100	704	4.40	-	-	DeWitt et al., 1989
Amphipod, <i>Eohaustorius estuarius</i>	fluoranthene	10 d LC50	3930	704	5.59	-	-	DeWitt et al., 1989
Amphipod, <i>Eohaustorius estuarius</i>	fluoranthene	10 d LC50	3570	704	5.07	5.00	5.46	DeWitt et al., 1989
Midge, <i>Chironomus tentans</i>	fluoranthene	10 d LC50	1590	704	-	-	-	Suedel et al., 1993
Midge, <i>Chironomus tentans</i>	fluoranthene	10 d LC50	1740	704	-	-	-	Suedel et al., 1993
Midge, <i>Chironomus tentans</i>	fluoranthene	10 d LC50	682	704	-	-	-	Suedel et al., 1993
Amphipod, <i>Diporeia</i> sp.	pyrene	31 d LC50	> 9090	694	> 13.1	-	-	Landrum et al., 1994
Amphipod, <i>Diporeia</i> sp.	fluoranthene	10 d LC50	(147000) > 23900 (29300)	704	> 34.0	> 34.0	> 34.0	Driscoll et al., 1997a

^A Bolded median response concentration (acute) values are the $C_{OC,PAH,MAX}$ based on the water solubilities of the PAH (Mackay et al., 1992). For these tests the interstitial water concentration at the median response concentration exceeded solubility. Therefore, solubilities are used instead of the acute value for further calculations.

^B Test-specific ESGUs: Quotient of the median response concentration ($\mu\text{g/goc}$) and $C_{OC,PAH,FCVI}$ (from Table 3-4).

^C PAH-specific SMAV: Geometric mean of the test-specific ESGTU_{FCVI} values from 10-d LC50 tests by species and PAH. Test-specific ESGTU_{FCVI} values greater than solubility included only if they are the sole 10-d LC50 for the species.

^D GMAV: Geometric mean of the PAH-specific SMAVs for all species within a genus.

^E Spiked sediments from Suedel et al. (1993) were unlikely at equilibrium; i.e., organisms were tested after only 18 to 24 hours after spiking.

Appendix E. Teratogenic effects from laboratory exposure to PAHs.

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
fathead minnow (embryos), <i>Pimephales promelas</i>	maternal via water	lab; flow-through	Anthracene	6.66 µg/L 11.6 µg/L	6 wks 3 wks	-yolk-sac malformations -edema -eye deformities	8.8a µg/g (eggs)	Effects on embryos incubated with solar ultraviolet light radiation	Hall and Oris, 1991
freshwater topminnows, <i>Poeciliopsis monacha</i> <i>Poeciliopsis lucida</i>	water; acetone carrier	lab; static renewal	BaP	1,000 µg/L nominal; 1,250 µg/L was acutely lethal	24 h followed by 6 mo. of monitoring	-increased AHH and EROD activities	9.0 µg/g converted from 35.7 nmol/g wet wt.	Implied effect - increased AHH and EROD activity indicative of carcinogenic and teratogenic metabolites formed during metabolism of BaP by MFO-system	Goddard et al., 1987
English sole (embryos), <i>Parophrys vetulus</i>	maternal via oral	lab; wild-caught	BaP	8,000 µg/L (8 mg/kg force-fed)	-	-malformation of tail regions -insufficient yolk-sac -reduced fin-fold size -reduced hatching success	51.2 and 263 µg/g (eggs) - avg. = 157; Tissue conc. from 80 mg/kg i.p. maternal injection	-Eggs maintained 11 days until yolk-sac absorbed; static. -Incidence of effect 4 times greater than controls (Chai-square df=3.81)	Hose et al., 1981
Rainbow trout (embryos), <i>Oncorhynchus mykiss</i>	aqueous from BaP spiked to sediment	lab; static renewal (7-10d)	BaP	0.21 µg/L measured	through to 36 d post-hatch	-nuclear pycnosis -lack of body pigment -insufficient yolk-sac -abnormalities of eyes -increased mortality (at 2.40 µg/L in aqueous) -muscle necrosis -abnormal mitosis in eyes and brains	1.93 µg/g (eggs), 12.34 µg/g (alevins), from exposure to 2.40 µg/L BaP	Poor control survival (52% mortality)	Hannah et al., 1982; Hose et al., 1984

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
Sand sole (embryos), <i>Psettiichthys melanostichus</i>	water; static	lab	BaP	0.1 µg/L measured; range (0.08 - 0.12)	through to yolk-sac absorption (7 -10 d)	-overgrowth of tissues -arrested development -twinning; Effects only after 48 h, i.e., during organogenesis	2.1 µg/g wet weight	effects only exhibited in 5% of animals; average hatching success of controls only 57% versus 28% BaP-treated	Hose et al., 1982
Flathead sole (embryos), <i>Hippoglossoides elassodon</i>	water; static	lab	BaP bound to bovine serum albumin	4.2 µg/L decreasing to <0.05 µg/L (DL)	through to yolk-sac absorption (7 -10 d)	-hatching success sig. decrease -nuclear pycnosis and general disruption of neural and ocular tissues	-	very low hatching success in controls and experimentals; 5.5 and 11.5%, respectively	Hose et al., 1982
English sole (embryos), <i>Parophrys vetulus</i>	water	lab	BaP	2.1 µg/L measured	through to yolk-sac absorption (7 -10 d)	none	-	-	Hose et al., 1982
gizzard shad, <i>Dorosoma cepedianum</i>	water via treated sediment	lab; static	BaP	1.38 µg/g sediment (initial); 0.74 µg/g sediment (mean of days 4,8 and 15)	22 d	none	BDL in all but 2 fish on day 4 - (0.001 and 0.0002 µg/g wet weight)	-40 ligated shad in 250 L H ₂ O with 4.15 kg sediment -no sig. decline in sediment conc. after day 4.	Kolok et al., 1996

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
gizzard shad, <i>Dorosoma cepedianum</i>	water and/or sediment ingestion	lab; static	BaP	1.02 µg/g sediment (initial); 0.63 µg/g sediment (mean of days 4, 8, and 15)	22 days	none	ligated fish: 0.010 µg/g wet weight (n=4) non-ligated: 0.012 µg/g wet weight (n=14)	-50 shad, 30 ligated; 20 non-ligated, in 500 L H ₂ O with 3.15 kg sediment -no sig. decline in sediment conc. after day 4 -all other tissue concs. BDL (n=26 ligated; n=6 non-ligated)	Kolok et al., 1996
estuarine clams, <i>Rangia cuneata</i>	water; acetone carrier	lab; static	BaP	30.5 µg/L	24 h	none	7.2 µg/g wet weight	-majority of BaP concentrated in the viscera (~75%) -n=5	Neff and Anderson, 1975
estuarine clams, <i>Rangia cuneata</i>	water; acetone carrier	lab; static	BaP	30.5 µg/L	24 h	none	5.7 µg/g wet weight	-majority of BaP concentrated in the viscera (~65%) -n=8	Neff and Anderson, 1975
coho salmon (24 h Post fertilization), <i>Oncorhynchus kisutch</i>	water; 0.5% DMSO	lab; static exposure then flow-through	BaP	25,000 µg/L	24 h	None	-	Effects on hatching, orientation, and foraging only.	Ostrander et al., 1988
coho salmon, (32 d post fertilization), <i>Oncorhynchus kisutch</i>	water; 0.5% DMSO	lab; static exposure then flow-through	BaP	25,000 µg/L	24 h	None	-	Effects on hatching, orientation, and foraging only.	Ostrander et al., 1988

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
coho salmon, (24 h Post fertilization), <i>Oncorhynchus kisutch</i>	water; 0.5% DMSO	lab; static exposure then flow-through	BaP	25,000 µg/L	24 h	None	0.54 decreasing to 0.15 nmol/mg protien from 2 to 68 d post fertilization	Conc. of BaP in tissue are not converted because wet weights were not given; only the mg protein/animal. Can possibly borrow weights from earlier paper.	Ostrander et al., 1989
coho salmon, (32 d post fertilization), <i>Oncorhynchus kisutch</i>	water; 0.5% DMSO	lab; static exposure then flow-through	BaP	25,000 µg/L	24 h	None	4.47 decreasing to 0.33 nmol/mg protien from 2 to 68 d post fertilization	Conc. of BaP in tissue are not converted because wet weights were not given; only the mg protein/animal. Can possibly borrow weights from earlier paper.	Ostrander et al., 1989
Calif. grunion (embryos), <i>Leuresthes tenuis</i>	water	lab; static	BaP	measured: 5 µg/L (steady-state); 24 µg/L (initial)	15 days	-reduction in % hatch -lateral folding of tail -absence of caudal fin folds -hemorrhagic lesion or congested vasculature in caudal region	day 15: 0.992 ppm (wet weight); 6.872 ppm (dry weight)	-steady state concentration reached in 4 to 10 days	Winkler et al., 1983

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
Calif. grunion (embryos), <i>Leuresthes tenuis</i>	water	lab; static	BaP	measured: 5-24 µg/L (steady state); 24-361 µg/L (initial)	15 days	-retarded growth (14d) -sporadic heart beat -displaced head relative to yolk-sac -absence of melanophores near lateral lines -absence of lens formation -lesions as larvae (above)	day 15: 0.92 to 10.48 µg/g wet weight; 6.87 to 62.80 µg/g (dry weight)	-steady state concentration reached in 4 to 10 days	Winkler et al., 1983
Calif. grunion (embryos), <i>Leuresthes tenuis</i>	water	lab; static	BaP	measured: 869 ppb (initial); steady-state not reached	15 days	-retarded growth (14d) -lateral curvature mid-body -absent melanophores -unused yolk sac -lesions as larvae (above)	day 15 - 19.98 µg/g wet weight; 112.03 µg/g dry weight	steady-state concentration never reached	Winkler et al., 1983
Pacific herring (embryos), <i>Clupea pallasii</i>	seawater contaminated by contact with oiled gravel - experiment 1; less weathered	lab; static	Field Mixture [^]	9.1 µ/L	16 days	-yolk sac edema	13.7 µg/g wet weight	Crude Oil characterized for PAHs only; concentrations of individual PAHs not given	Carls et al., 1999

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
Pacific herring (embryos), <i>Clupea pallasii</i>	seawater contaminated by contact with oiled gravel - experiment 2; more weathered	lab; state	Field Mixture ^A	0.41 µ/L to 0.72 µ/L	16 days	- yolk sac edema - pericardial edema - skeletal, spinal, and craniofacial abnormalities - anaphase aberration	0.022 µg/g wet weight	Crude Oil characterized for PAHs only; concentrations of individual PAHs not given	

^A Artificially weathered Alaska North Slope crude oil.

Appendix F. Carcinogenic effects from laboratory and field exposure to PAHs and PAH mixtures.

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
Japanese Medaka, <i>Oryzias latipes</i> (6-10 d old)	Water; dimethyl-formamide carrier.	Lab; static	BaP	261 µg/L	2 x 6h, 1 week apart	Neoplastic lesions in livers and other tissues after 36 weeks 36% vs 1% (controls); 20 fish with adenoma, 6 with hepatocellular carcinoma		Exposures carried out at 26°C in the dark; concentration exceeds saturation solubility of BaP	Hawkins et al, 1988; Hawkins et al., 1990
guppy, <i>Poecilia reticulata</i> (6-10 d old)	Water; dimethyl-formamide carrier.	Lab; static	BaP	209 µg/L	2 x 6h, 1 week apart	Neoplastic lesions in livers and other tissues after 52 weeks 23% vs 0% (controls); 1 altered foci, 5 adenoma, 4 with hepatocellular carcinoma		Studies carried out longer because tumorigenic response in guppy is slower than in medaka	Hawkins et al, 1988; Hawkins et al., 1990
Rainbow trout (fingerlings), <i>Oncorhynchus mykiss</i>	oral	Lab	BaP	1,000 ppm per feeding	12 and 18 months	Incidence of neoplasms on liver 15% (1.0/liver) at 12 months 25% (7.7/liver) at 18 months	-	MFO info also available 0% at 6 months 0% on other organs	Hendricks et al., 1985
Rainbow trout (juvenile), <i>Oncorhynchus mykiss</i> (10 mo)	ip injection	Lab	BaP	1 mg B(a)P in 0.4 ml PG (1/month for 12 months)	18 months (6 months after final injection)	Incidence of neoplasms in various organs = 46% (x = 7.7 tumors/organ)	-	Organs examined = gonads, swim bladder, liver, spleen, head and trunk kidneys, pancreas, intestines, and stomach	Hendricks et al., 1985

Species	Mode of Exposure	Method	PAH	Exposure Conc Associated with Effect	Exposure Time	Toxic Effect(s):	Tissue Conc	Comments:	Reference
<i>Poeciliopsis lucida</i> and <i>Poeciliopsis monacha</i> (1-7 months old)	water; acetone carrier	Lab: (multiple exposures) 3 to 4 exposure periods of 5-20 hours each week	7,12-dimethylbenz(a)-anthracene	5 ppm (per exposure)	7 - 8 months (from initial exposure)	incidence of hepatic tumors = 48%	-	only survivors examined = (55% mortality in 5 ppm treatment) (13% mortality in control)	Schultz and Schultz 1982
<i>Poeciliopsis lucida</i> and <i>Poeciliopsis monacha</i> (1-6 weeks old)	water; acetone carrier	Lab: (multiple exposures) 5 exposures periods of 6 hours each week	7,12-dimethylbenz(a)-anthracene	5 ppm (per exposure)	6 - 7 months	Incidence of hepatic tumors = 41.8%	-	22% mortality in treatment 16% mortality in control Tumor-bearing livers enlarged, yellow-white to greenish and granular.	Schultz and Schultz 1982
Bullheads	Direct skin (river sediment extract)	Lab	Field Mixture ^A	5% RSE painted once per week	18 months	23% of survivors hyperplastic 9% with multiple papillomas	-	Survival of control and experimental fish was 31%.	Black, 1983
Japanese Medaka, <i>Poecilia reticulata</i> (6-10 d old)	Water via Sediment extract re-dissolved in acetone	Lab	Field Mixture ^B	182 ppb TPAH Black River, OH extract; 254 ppb TPAH Fox River, WI extract	24 h	hepatocellular carcinoma - Black River Ex. (2/15 fish); Pancreatic-duct cell adenoma - Fox River Ex. (1/15 fish)	-	No incidence of carcinomas in controls up to 270 days post-exposure; one incidence of lymphoma after 360 days of exposure.	Fabacher et al., 1991
Rainbow trout (embryos), <i>Oncorhynchus mykiss</i>	injection of sediment extract into yolk sac	Lab	Field Mixture ^C	Doses ^D : (Exp I) 0.006 g (Exp II) 0.012 g 0.006 g 0.003 g	1 year	Hepatic carcinomas (I) 8.9% (11/123) (II) 8.1% (12/148) 4.0% (5/148) 3.1% (2/65)	-	Note; PCBs also present sediment from Hamilton Harbour	Metcalfe et al 1988

Buffalo River, NY; total no. PAHs measured = 13, total no. of carcinogenic PAHs = 6.

Black River, OH. And Fox River, WI; full compliment of measured PAHs.

Hamilton Harbor, ON, Canada; total no. PAHs measured = 13, total no. of carcinogenic PAHs = 6.

Doses are calculated as gram equivalent wet weight of sediment represented by the volume of extract micro-injected into each trout sac-fry.

FIGURES

- Figure 2-1. Schematic diagram of the $\log_{10}\text{LC50}$ versus $\log_{10}K_{\text{OW}}$ relationship. At $\log_{10}K_{\text{OW}} = 0$, $K_{\text{OW}} = 1$, the concentration in water equals the concentration in octanol.
- Figure 2-2. Comparisons of (A) $\log_{10}K_{\text{OW}}$ predicted by SPARC versus measured $\log_{10}K_{\text{OW}}$ using slow stir method and (B) reported $\log_{10}\text{LC50}$ values versus the aqueous solubility estimated by SPARC. The diagonal line represents equality.
- Figure 2-3. Ratios of (A) 48- to 96-hour LC50 values and (B) 24- to 96-hour LC50 values versus $\log_{10}K_{\text{OW}}$. The line in (B) is the regression used to correct the 24-hour LC50 to 96-hour LC50.
- Figure 2-4. $\log_{10}\text{LC50}$ versus $\log_{10}K_{\text{OW}}$ for the indicated species. The line has a constant slope of -0.945 . The y-intercepts vary for each species. Outliers are denoted by a plus symbol (+).
- Figure 2-5. Statistical comparison of slopes fitted to individual species to the universal slope of -0.945 showing (A) the probability that the difference occurred by chance (filled bars) and number of data points in the comparison (hatched bars) for each species in the database, and (B) the deviations of the individual estimates from the universal slope. Abbreviations are based on the first letter of the genus and either the first or second letters of the species names given in Appendix A (e.g., *Aae* = *Aedes aegypti* and *Am* = *Ambystoma mexicanum*).

Figure 2-6. Chemical class comparisons. (A) Residuals from the regression grouped by class with mean \pm 2 standard errors. (B) Residuals grouped by class with chemical class corrections included in the regression.

Figure 2-7. The coefficient of variation of the estimated species-specific body burdens versus the number of data points for that species (A), the log probability plot of the residuals (B), and the residuals versus $\log_{10}K_{ow}$ (C).

Figure 2-8. $\log_{10}LC50$ versus $\log_{10}K_{ow}$ for (A) *L. macrochirus*, (B) *D. pulex*, and (C) *G. affinis*. The line connects the individual estimates of the LC50 values, including the chemical class correction.

Figure 2-9. Comparison of target lipid model, line-of-fit and observed LC50 data for individual PAHs, by species. The PAHs included are: naphthalene (3.36), 1-methylnaphthalene (3.84), 2-methylnaphthalene (3.86), 2-chloronaphthalene (3.88), 1-chloronaphthalene (3.88), acenaphthene (4.01), phenanthrene (4.57), pyrene (4.92), 9-methylanthracene (5.01), fluoranthene (5.08). Number in parentheses = $\log_{10}K_{ow}$. Solid line and filled symbols are for non-halogenated PAHs. Dotted lines and unfilled symbols are for the halogenated (i.e., chlorinated) PAHs. Plus symbols (+) denote outliers. Data are from Di Toro et al. (2000) and were used for toxicity test screening criteria.

Figure 2-10. Predicted and observed body burdens for five species.

Figure 2-11. Additivity of type I narcosis toxicity. Comparison of the observed TU concentrations calculated from four studies to the predicted TU of 1.0. The number of chemicals in

the tested mixtures are as indicated (adopted from Hermens et al., 1984).

Figure 3-1. GMAVs at a $\log_{10}K_{ow}$ of 1.0 from water-only acute toxicity tests using freshwater and saltwater genera versus percentage rank of their sensitivity. Freshwater genera are indicated by open symbols and saltwater genera are indicated by closed symbols.

Figure 3-2. Probability distributions of FAV difference statistics to compare water-only toxicity data from (A) freshwater versus saltwater genera and (B) benthic versus WQC.

Figure 4-1. Probability distribution of the $\Sigma ESGTU_{FCV}$ for PAH mixtures in sediments from coastal and estuarine locations in the United States (NOAA, 1991; Adams et al., 1996; Anderson et al., 1996; Fairey et al., 1996; U.S. EPA, 1996a, b, 1998; Hunt et al., 1998). Horizontal line indicates a toxic unit of 1.0.

Figure 4-2. Probability distribution of the $\Sigma ESGTU_{FCV}$ for PAH mixtures in sediments from all the coastal and estuarine locations in the United States from Figure 4-1 (NOAA, 1991; Adams et al., 1996; Anderson et al., 1996; Fairey et al., 1996; U.S. EPA, 1996a, b, 1998; Hunt et al., 1998). Horizontal line indicates a toxic unit of 1.0.

Figure 5-1. Percent mortality versus predicted interstitial water toxic units for six chemicals and three sediments per chemical. Sediment types are indicated by open symbols (lowest organic carbon content), doubled symbols (intermediate organic carbon content) and filled symbols (highest organic carbon content).

Figure 5-2. Percent mortality versus predicted interstitial water toxic units for seven chemicals and

three sediments per chemical. Sediment types are indicated by open symbols (lowest organic carbon content), doubled symbols (intermediate organic carbon content) and filled symbols (highest organic carbon content). Uncertainty error bars are represented by solid vertical lines (see U.S. EPA, 1999a for source of K_{OC} values).

Figure 5-3. Percent mortality of *Rhepoxynius abronius* in sediments spiked with acenaphthene, phenanthrene, fluoranthene, or pyrene (see Appendix D for data).

Figure 5-4. Percentage rank, based on $ESGTU_{FCVI}$, of the sensitivities of genera of benthic organisms from spiked sediment toxicity tests with individual PAHs.

Figure 5-5. Mortality of the amphipod, *Rhepoxynius abronius*, from tests 10-day sediment toxicity tests with four parent PAHs separately (triangles) and in combination (circles) from (Swartz et al., 1997) versus predicted sediment toxic units (PSTUs). PSTUs are the sediment concentrations in each treatment divided by the predicted PAH-specific sediment LC50 values. The predicted PAH-specific sediment LC50 values are derived from the interstitial water 10-day LC50 values from spiked sediment toxicity tests and the universal narcosis slope to derive the PAH-specific critical tissue concentrations. The geometric mean of the critical tissue concentrations, the universal narcosis slope and the PAH-specific K_{OW} and K_{OC} were used to derive PAH-specific sediment LC50 values. For the mixture experiment the toxic units are the sum of the sediment concentrations for each of the four PAHs divided by their respective PAH-specific sediment LC50 values.

Figure 5-6. Response of *H. azteca* exposed for 10 days under flow-through conditions to sediment

spiked with a mixture of high K_{ow} PAH. Acute TUs were calculated based on measured sediment PAH concentrations and the GMAV from Appendix C. Asterisks indicate significant reduction compared to the control ($\alpha=0.05$).

Figure 5-7. Response of *H. azteca* exposed for 28 days under flow-through conditions to sediment spiked with a mixture of high K_{ow} PAH. Acute TUs were calculated based on measured sediment PAH concentrations and the GMAV from Appendix C. Asterisks indicate significant reduction compared to the control ($\alpha=0.05$).

Figure 5-8. Survival (after 28 days) and growth (after 10 days) of *H. azteca* expressed on the basis of measured PAH concentrations in tissues (lipid normalized). Effect concentrations were calculated from acute water-only effect data for fluoranthene, methanol, ethanol, and 2-propanone using the narcosis model. Acute TUs were calculated by dividing the lipid-normalized concentration of PAH in tissue by the GMAV, assuming lipid \approx octanol. The chronic threshold is represented by the GMAV divided by the ACR. Data are from Di Toro et al. (1999).

Figure 5-9. Response of *H. azteca* exposed for 10 days (3 renewals) to sediment spiked with a mixture of high K_{ow} PAH. Acute TUs were calculated based on measured sediment PAH concentrations and the GMAV from Appendix C. Asterisks indicate significant reduction compared to the control ($\alpha=0.05$).

Figure 5-10. Response of *L. plumulosus* exposed for 10 days under static conditions to sediment spiked with a mixture of high K_{ow} PAH. Acute TUs were calculated based on measured sediment PAH concentrations and the GMAV from Appendix C. Asterisks

are treatments with effects significantly different from controls.

Figure 5-11. Amphipod (*Ampelisca abdita*) abundance versus $\Sigma\text{ESGTU}_{\text{FCV}}$. Vertical line is the ESG of 1.0 $\Sigma\text{ESGTU}_{\text{FCV}}$. Data are from the Virginian and Louisianian province EMAP (U.S. EPA, 1996a,b) and the New York/New Jersey Harbor REMAP (Adams et al., 1996).

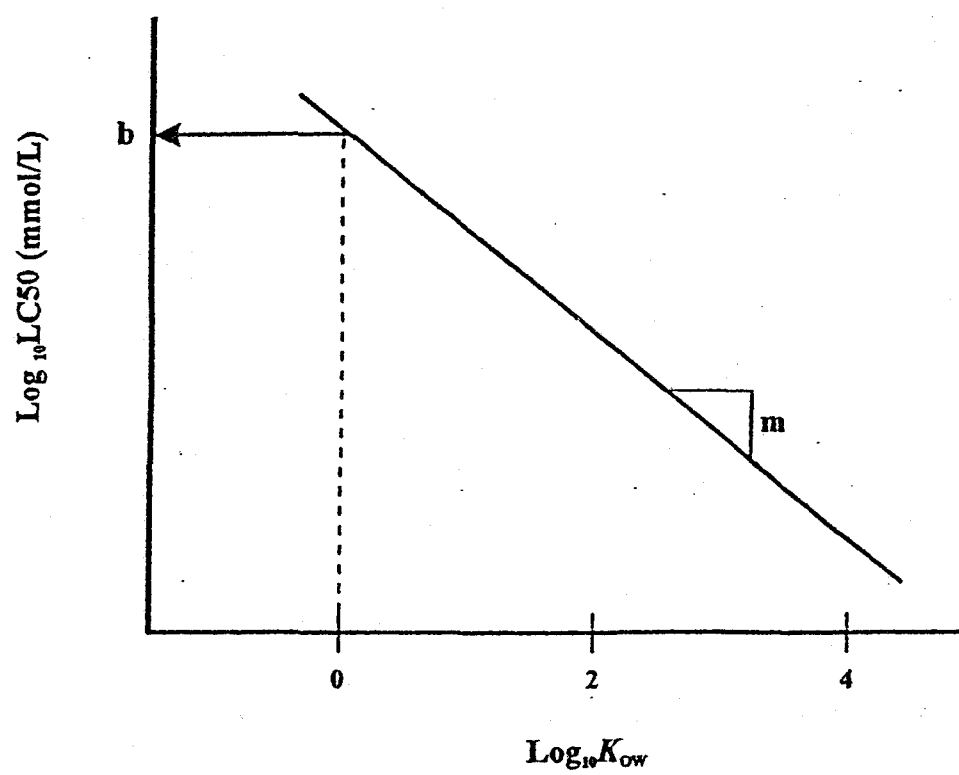
Figure 6-1. Comparison of observed $\Sigma\text{ESGTU}_{\text{FCV,TOT}}$ to observed $\Sigma\text{ESGTU}_{\text{FCV,13}}$ from 13 PAHs (A) and $\Sigma\text{ESGTU}_{\text{FCV,23}}$ from 23 PAHs (B) for the combined dataset including U.S. EPA EMAP Louisian and Carolinian Provinces (N=490). The line shows the resulting log-log linear regression equation.

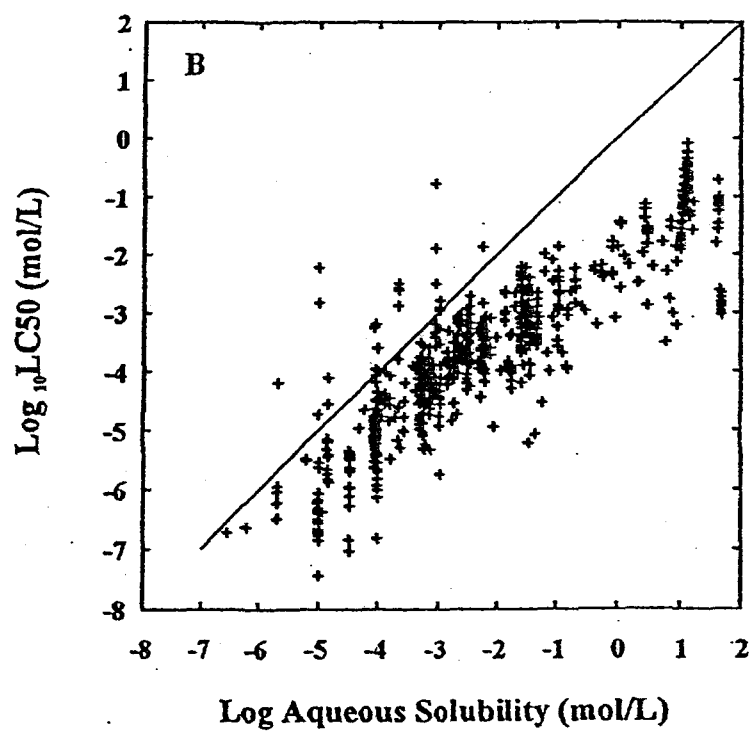
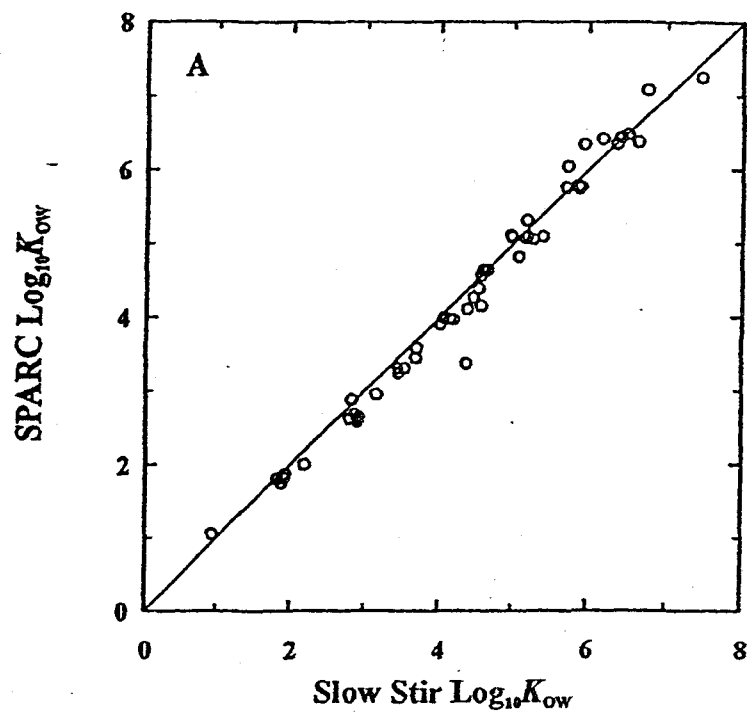
Figure 6-2. Probability distribution of the (A) $\Sigma\text{ESGTU}_{\text{FCV,13}}$ and (B) $\Sigma\text{ESGTU}_{\text{FCV,23}}$ values for each sediment from the entire database. Symbols are as described in text.

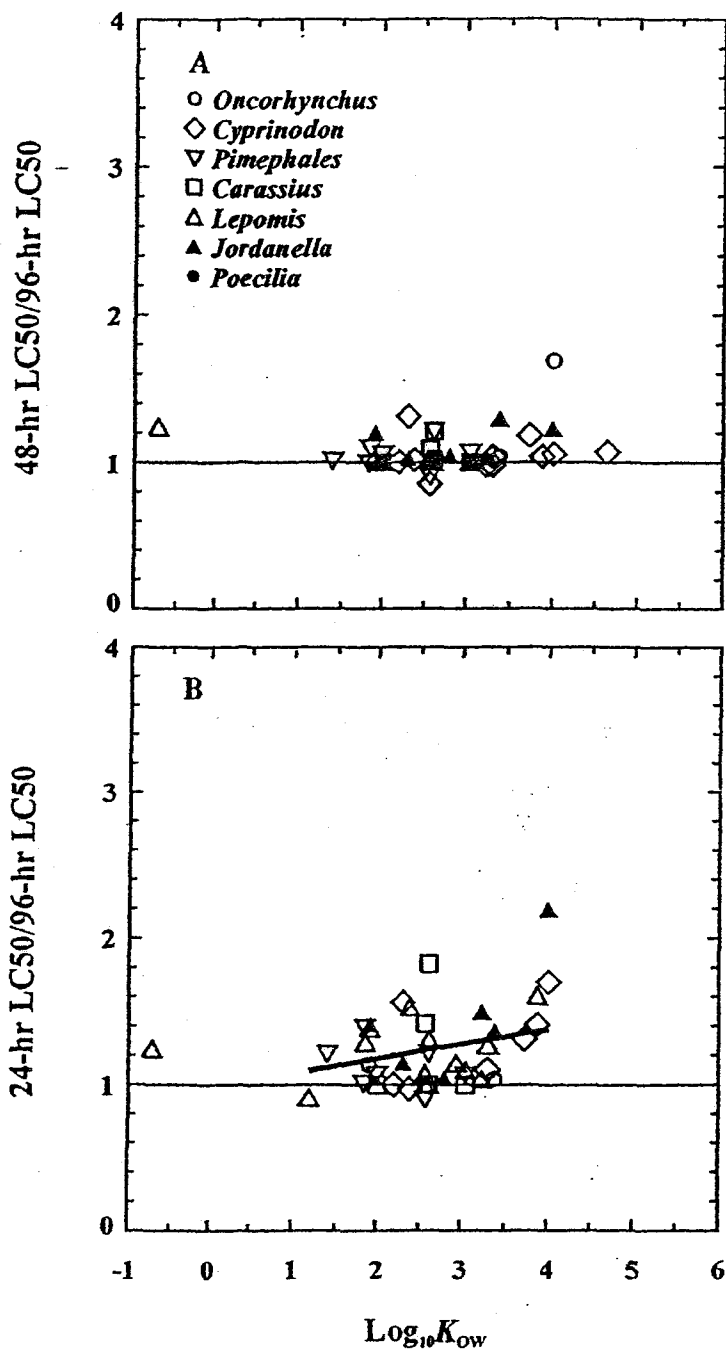
Figure 6-3. BaP concentration of 539 sediment samples from the EMAP and Elliot Bay datasets versus the ΣESGUs of 34 PAHs (A) and a probability plot of these BaP concentrations at an $\Sigma\text{ESGU} = 1$ (B). The solid line in both plots is the BaP critical sediment concentration for teratogenic and carcinogenic effects ($57 \mu\text{g/g}_{\text{OC}}$).

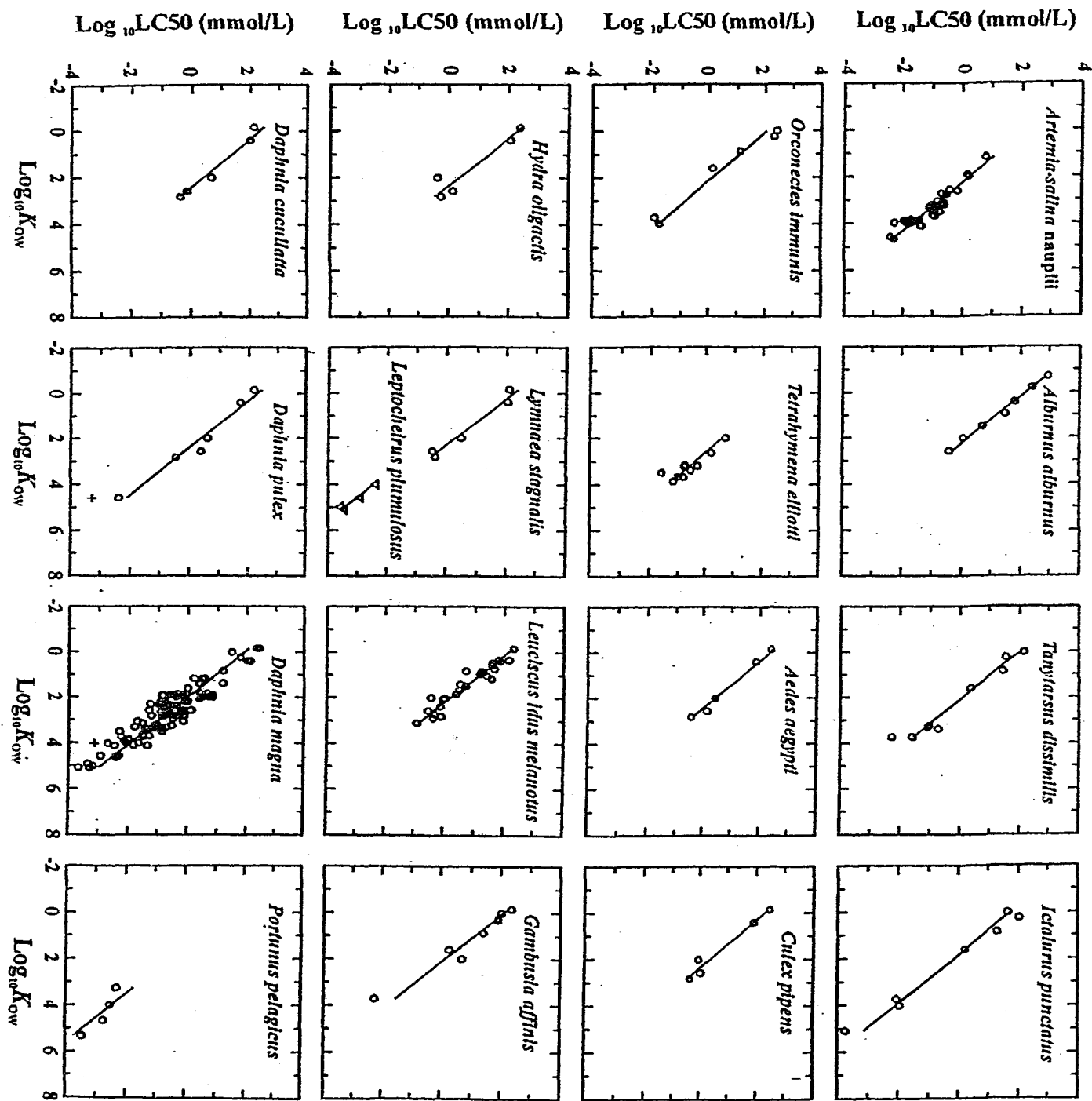
Figure 6-4. Anthracene concentration of 539 sediment samples from the EMAP and Elliot Bay datasets versus the ΣESGUs of 34 PAHs (A) and a probability plot of these Anthracene concentrations at an $\Sigma\text{ESGU} = 1$ (B). The solid line in both plots is the Anthracene critical sediment concentration for teratogenic effects ($219 \mu\text{g/g}_{\text{OC}}$).

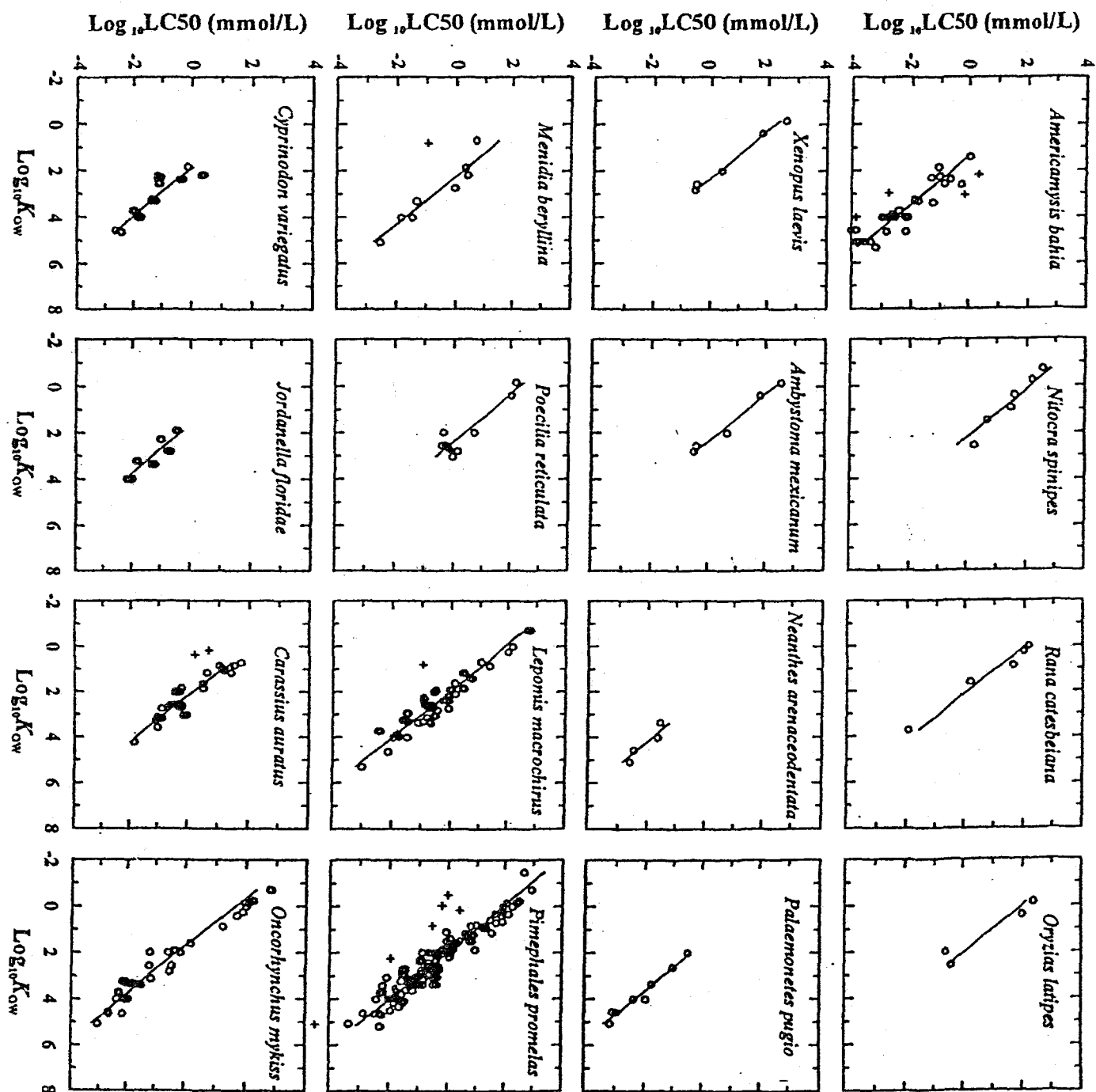
Figure 6-5. Computed solubilities of nine PAHs relative to their 25°C solubilities as a function of temperature. The solid line is the least-squares regression line (Equation 6-10).

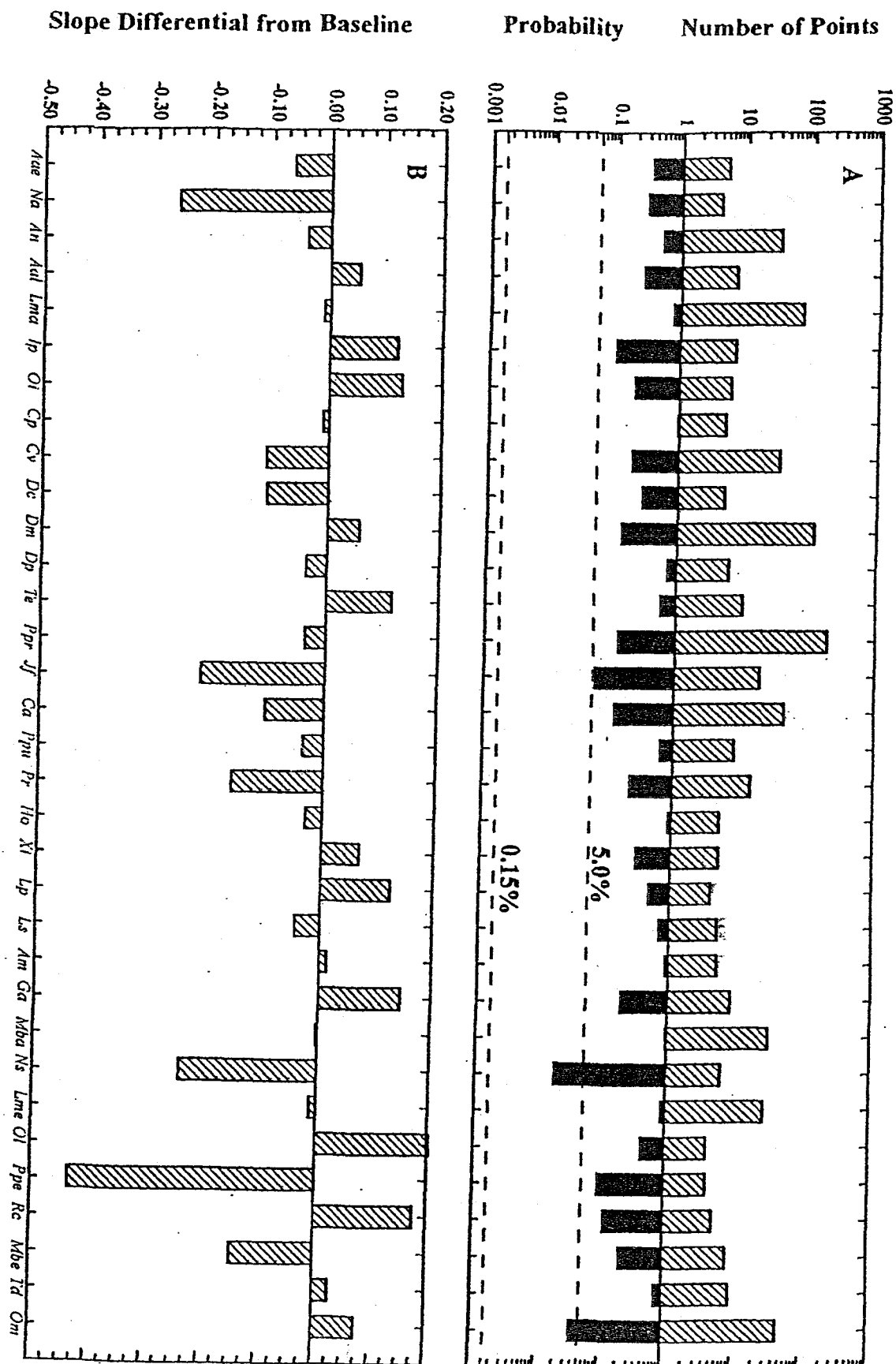




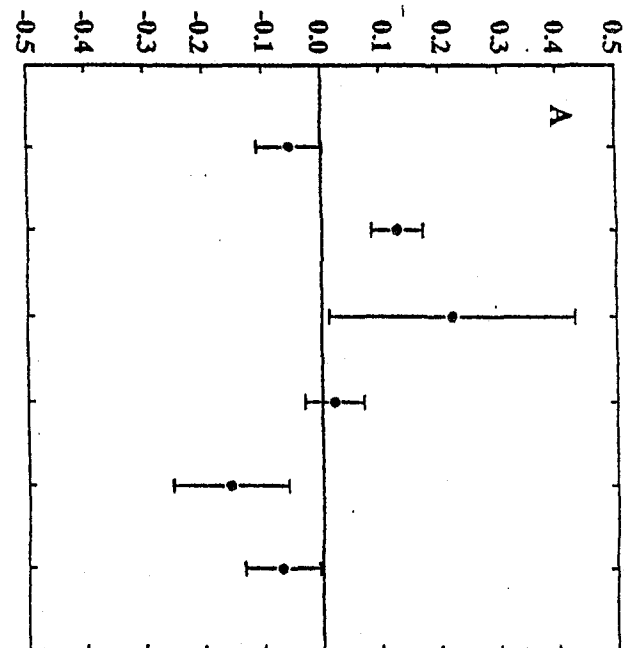




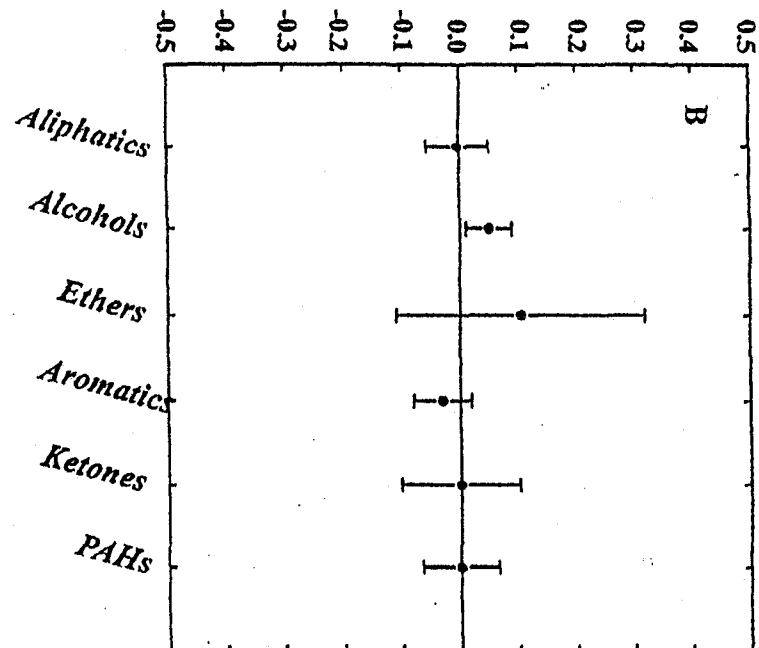


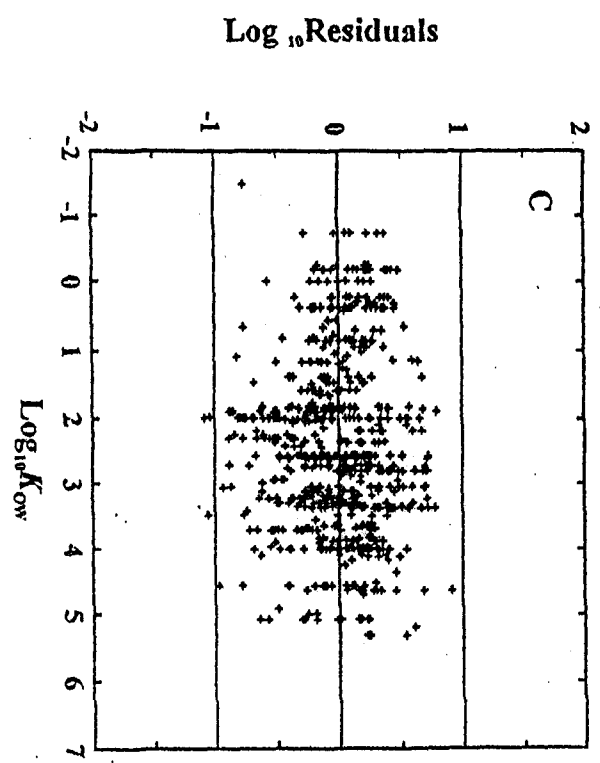
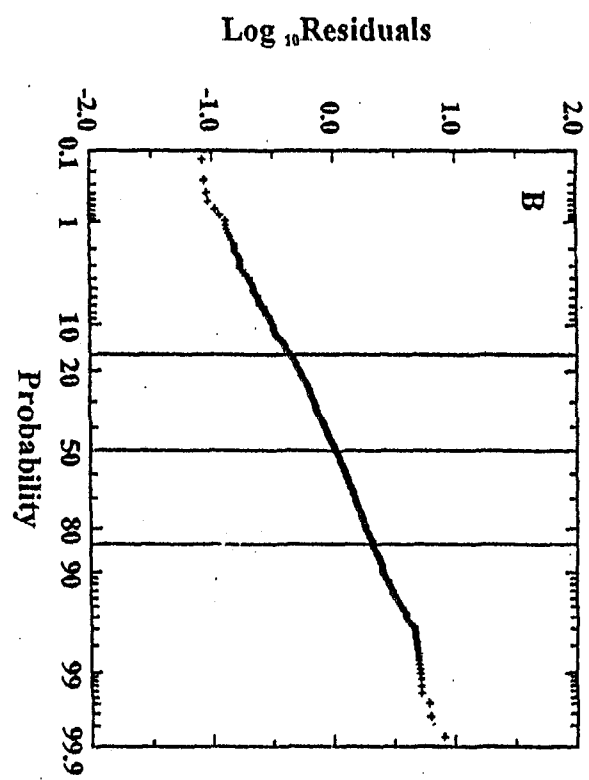
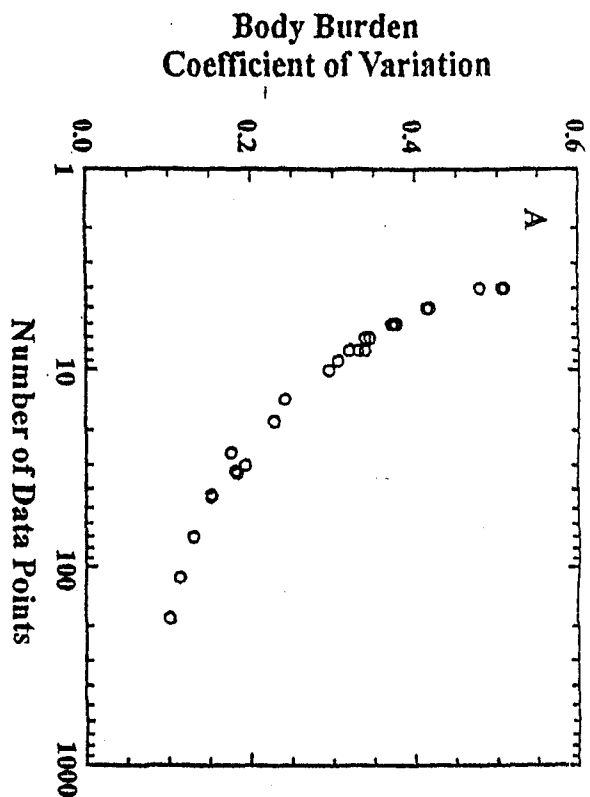


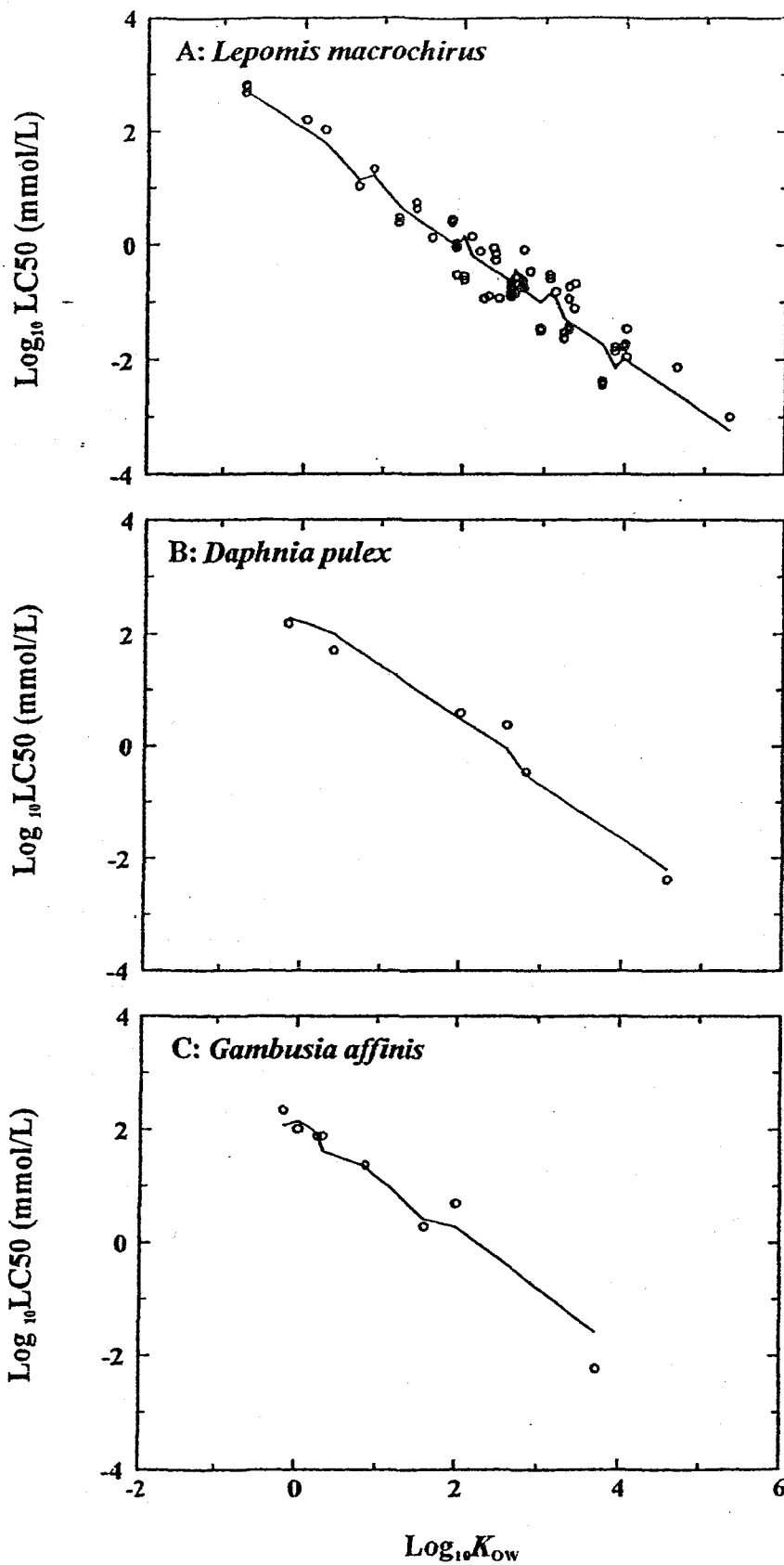
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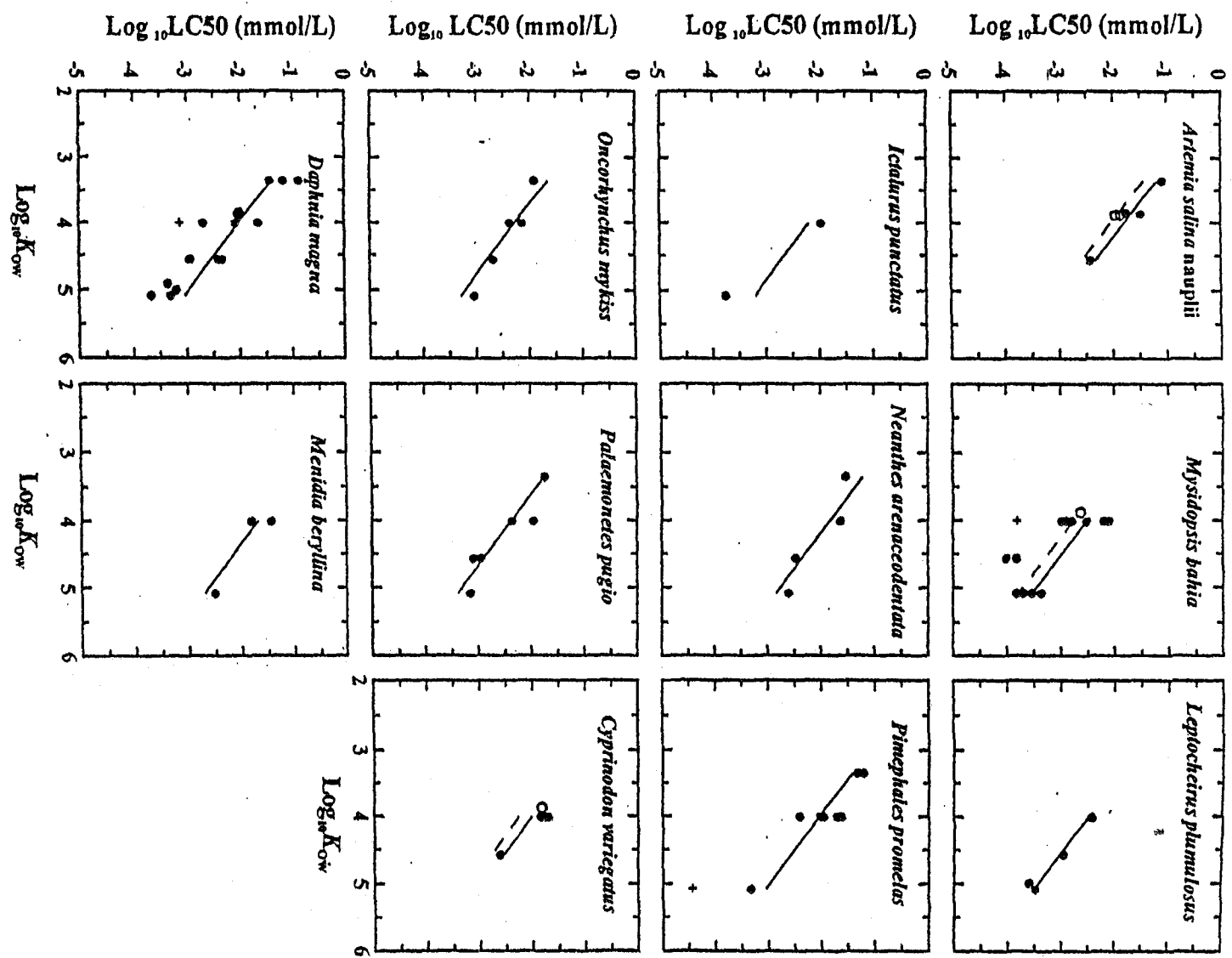


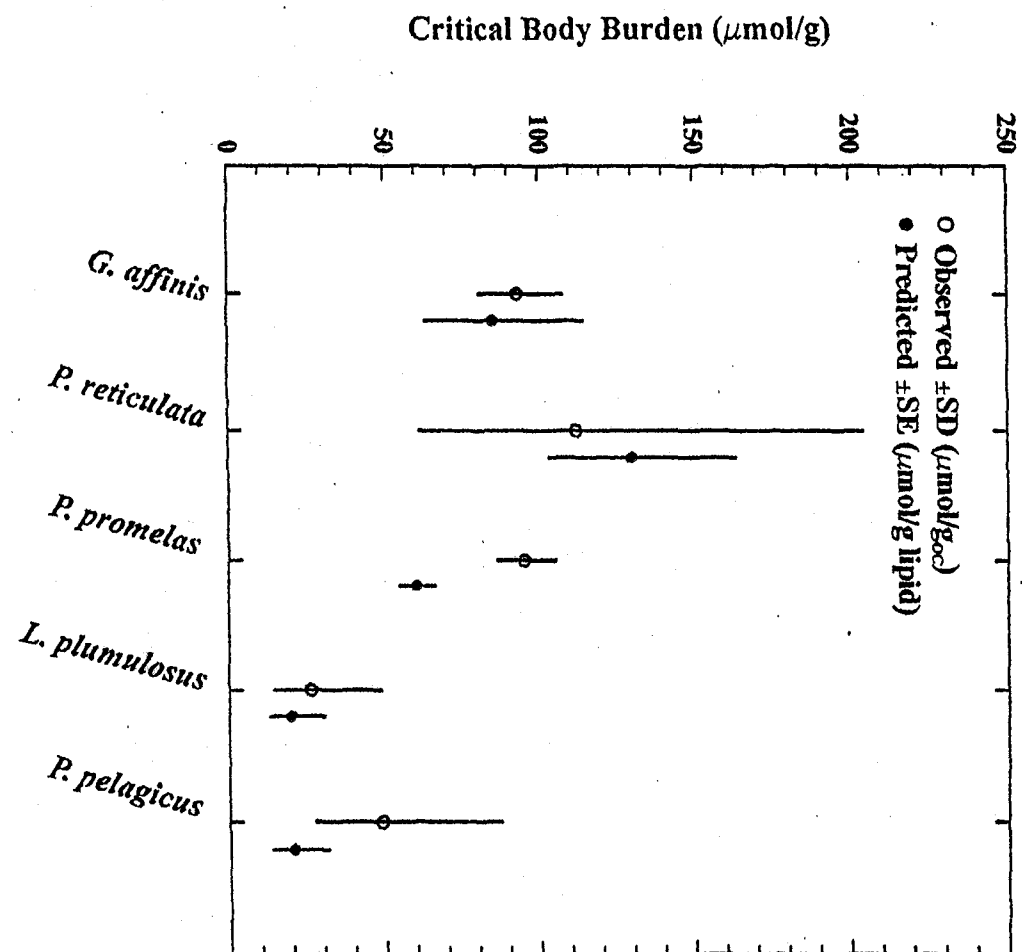
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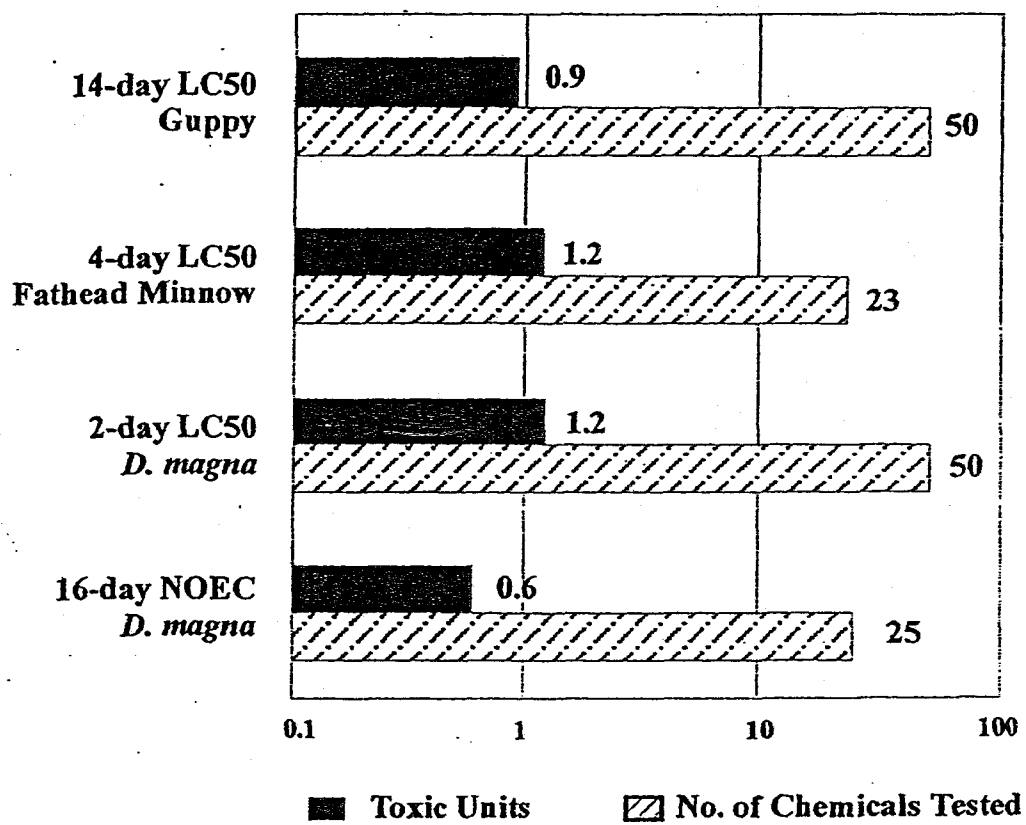


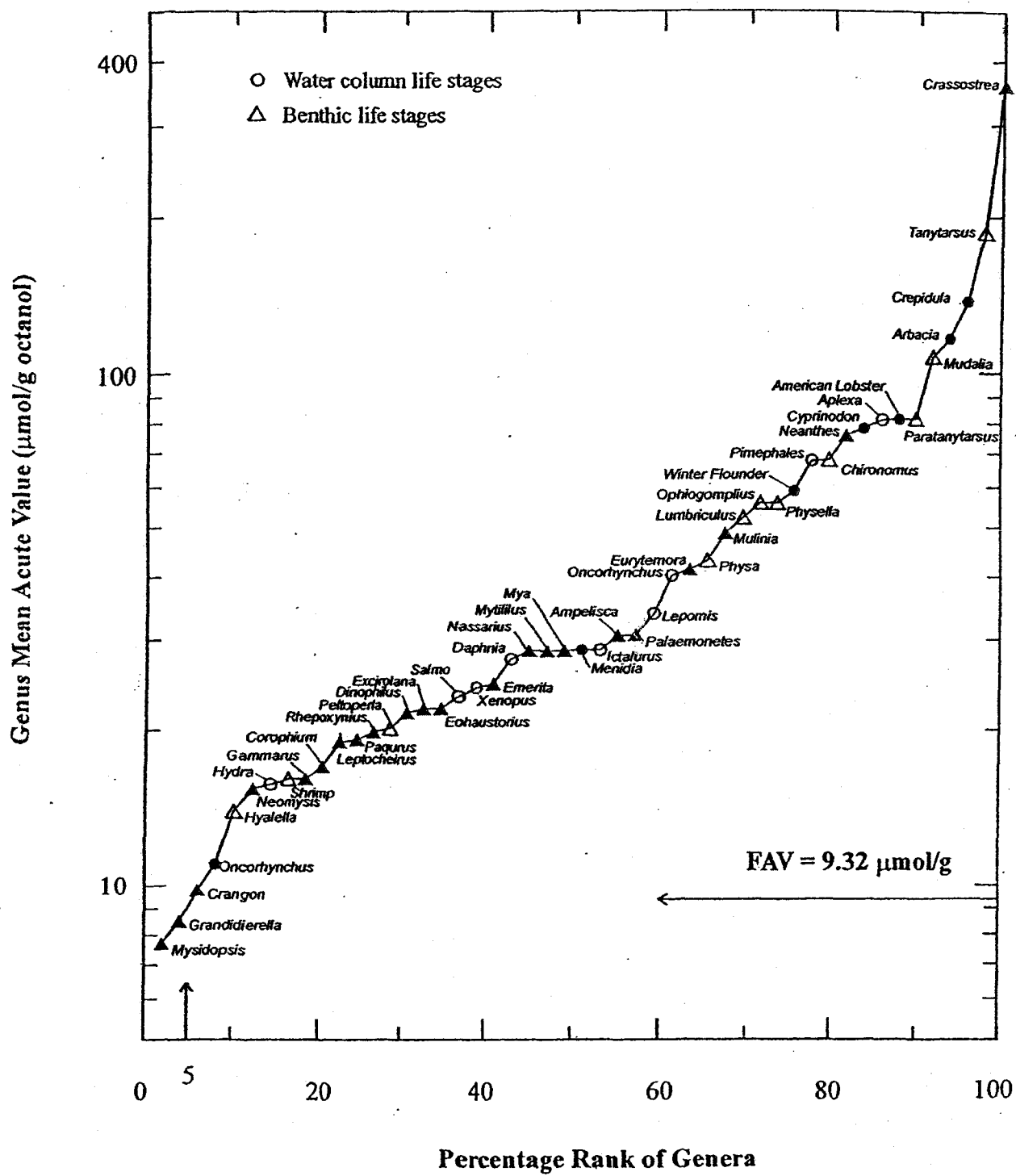


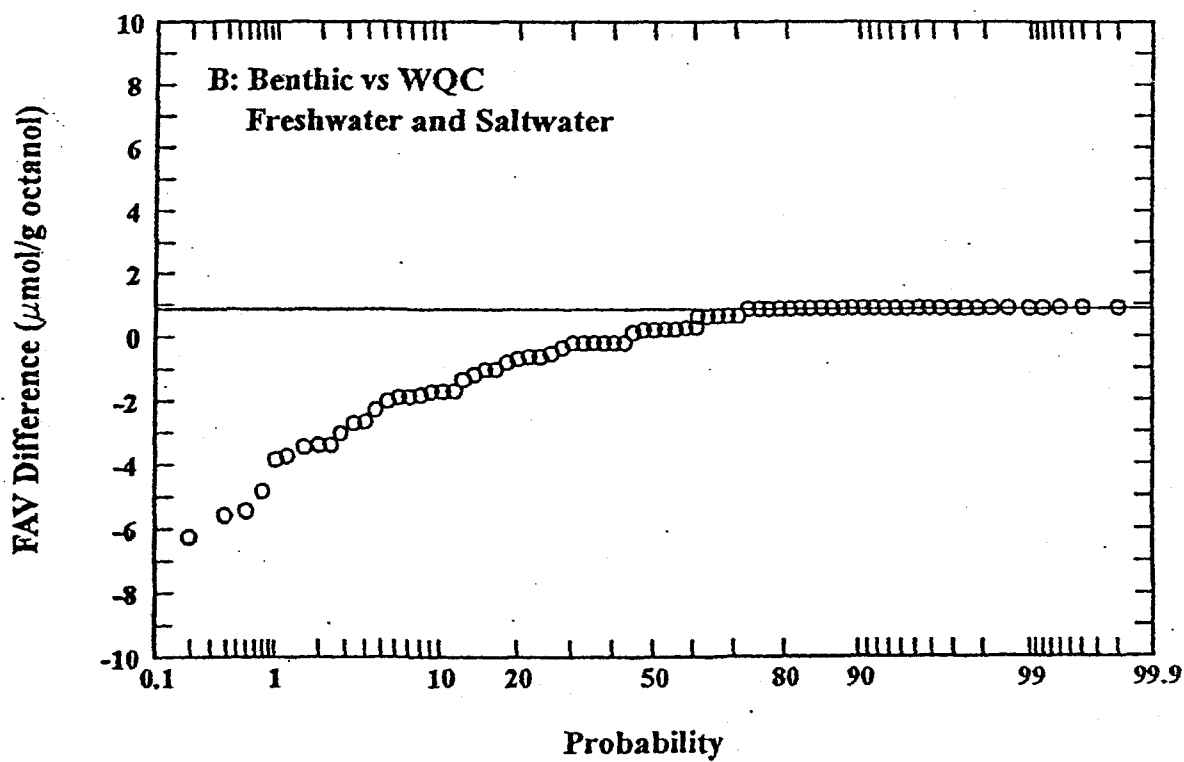
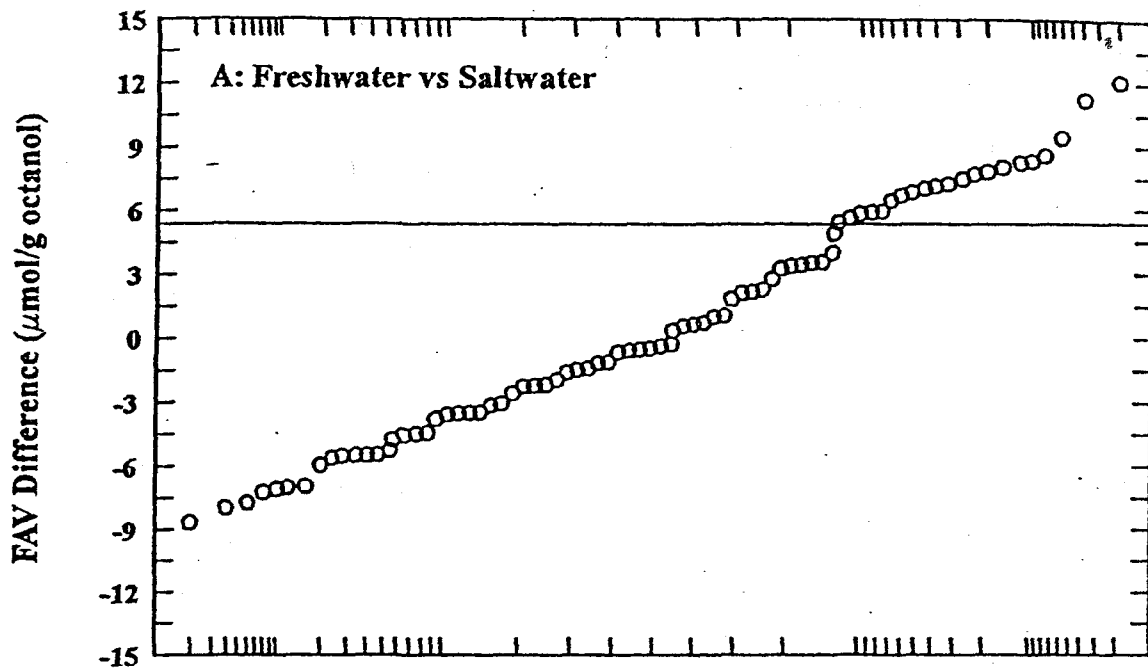


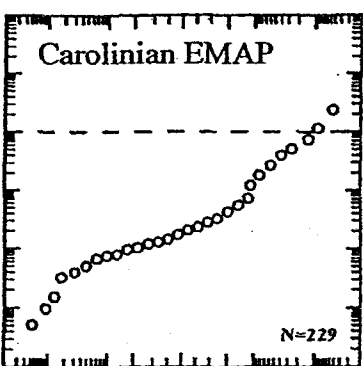
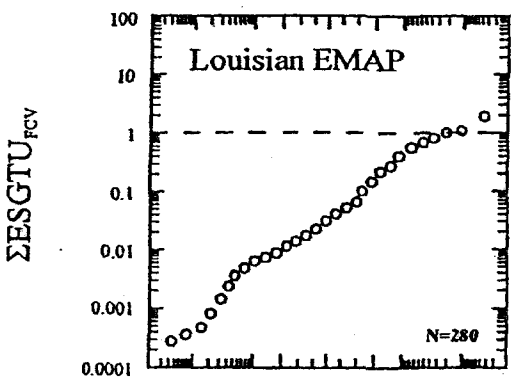
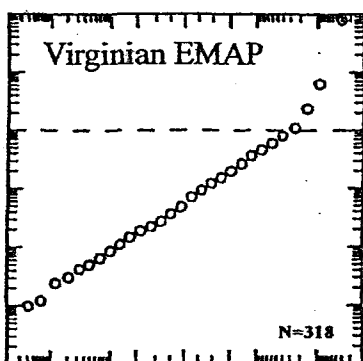
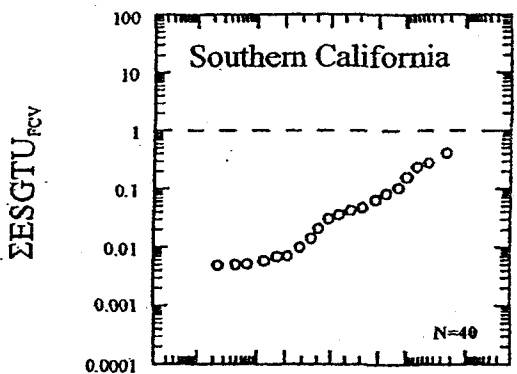
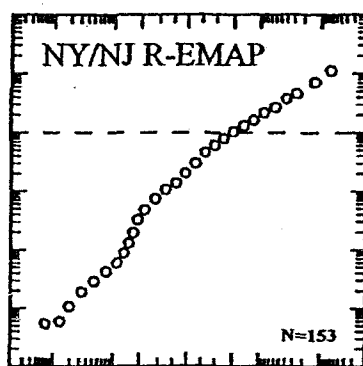
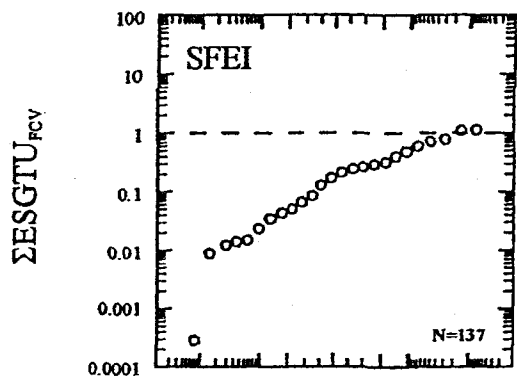
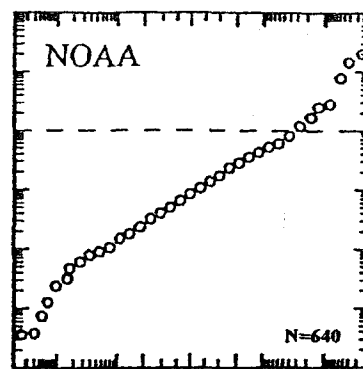
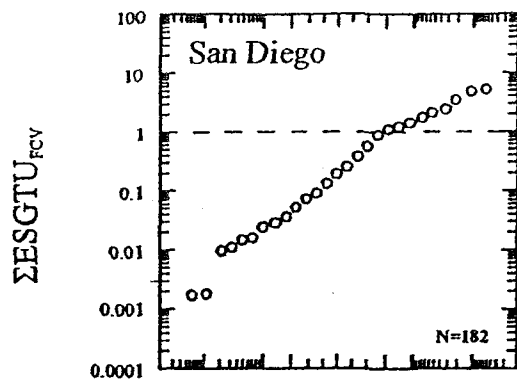






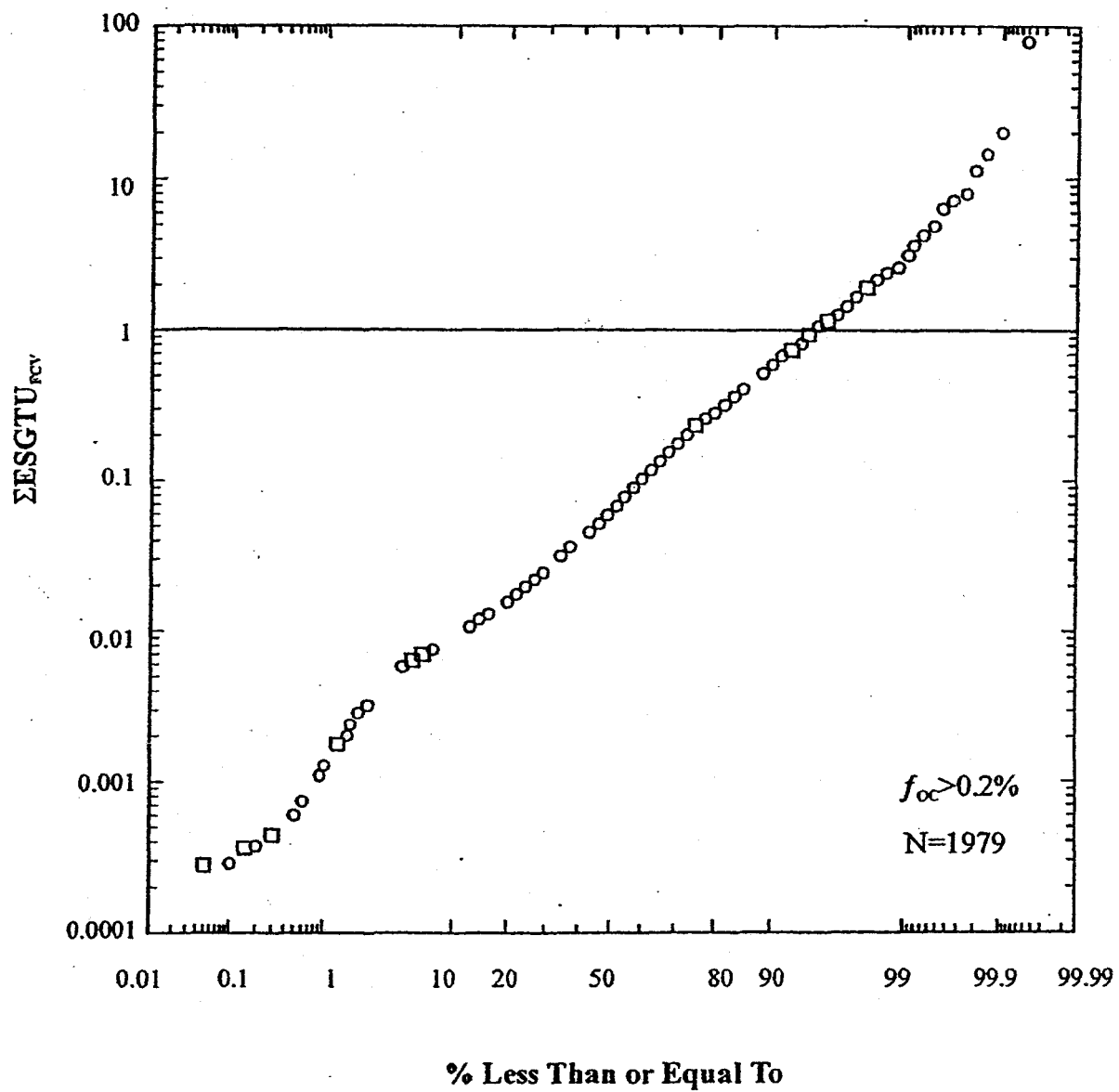


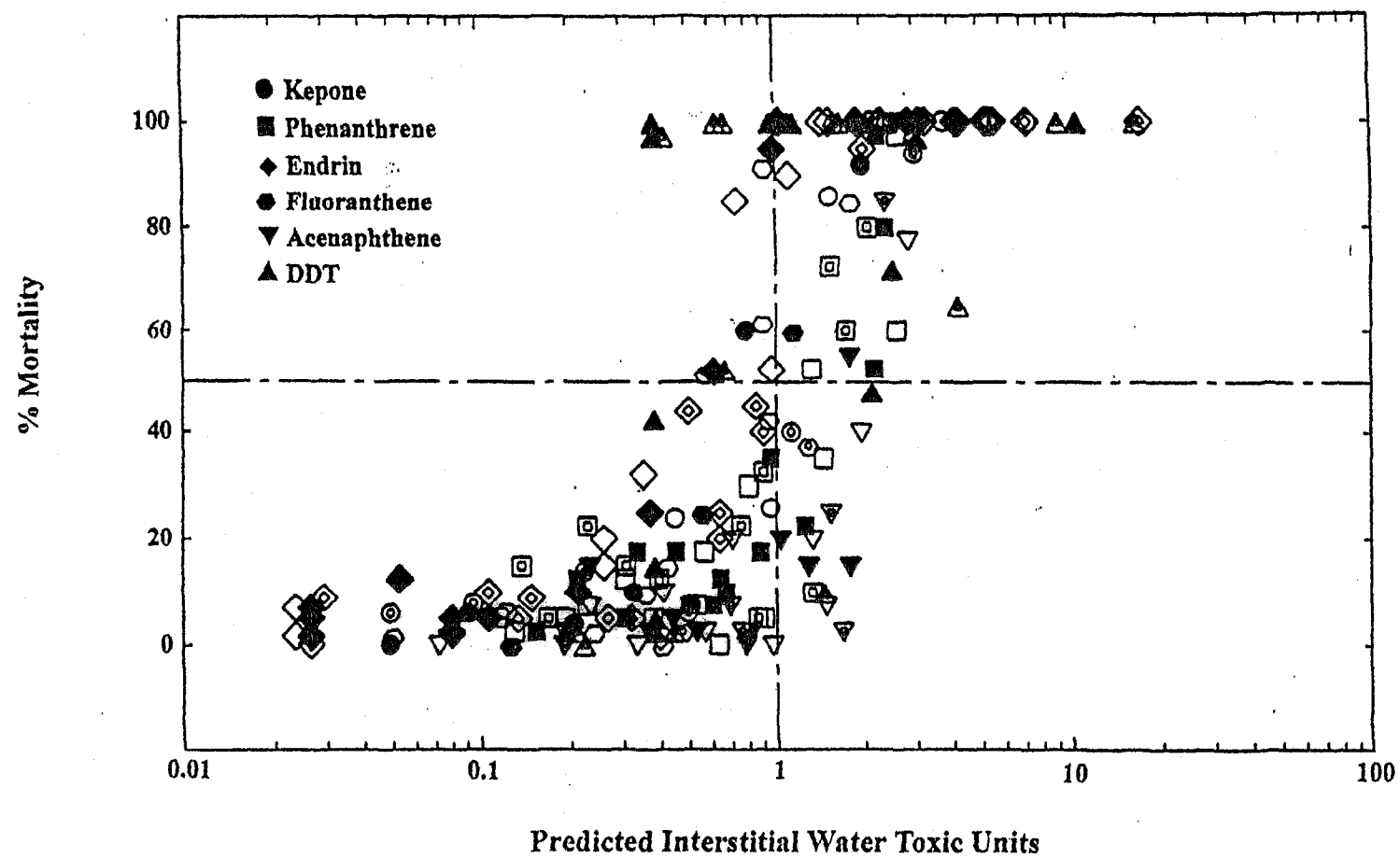


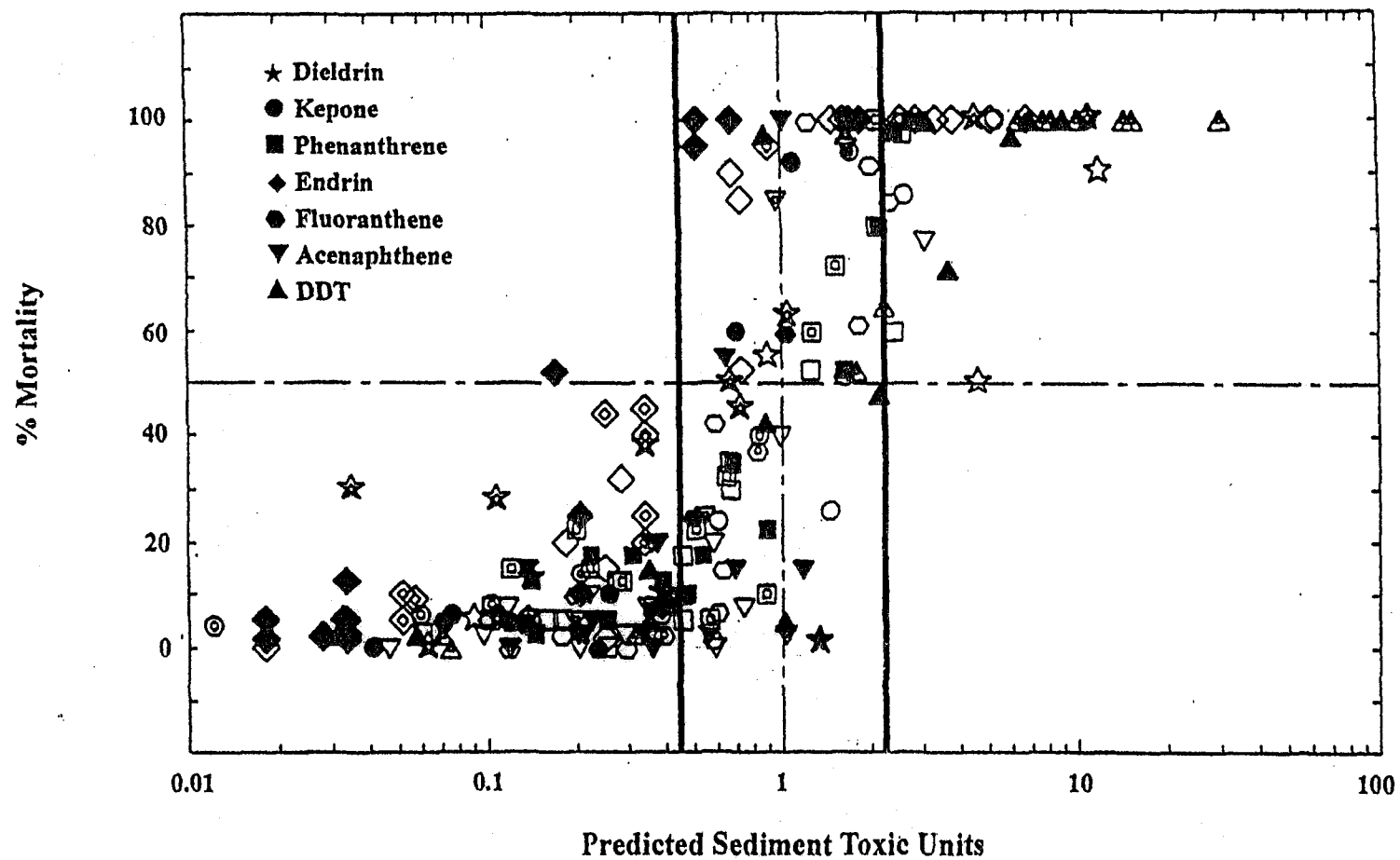


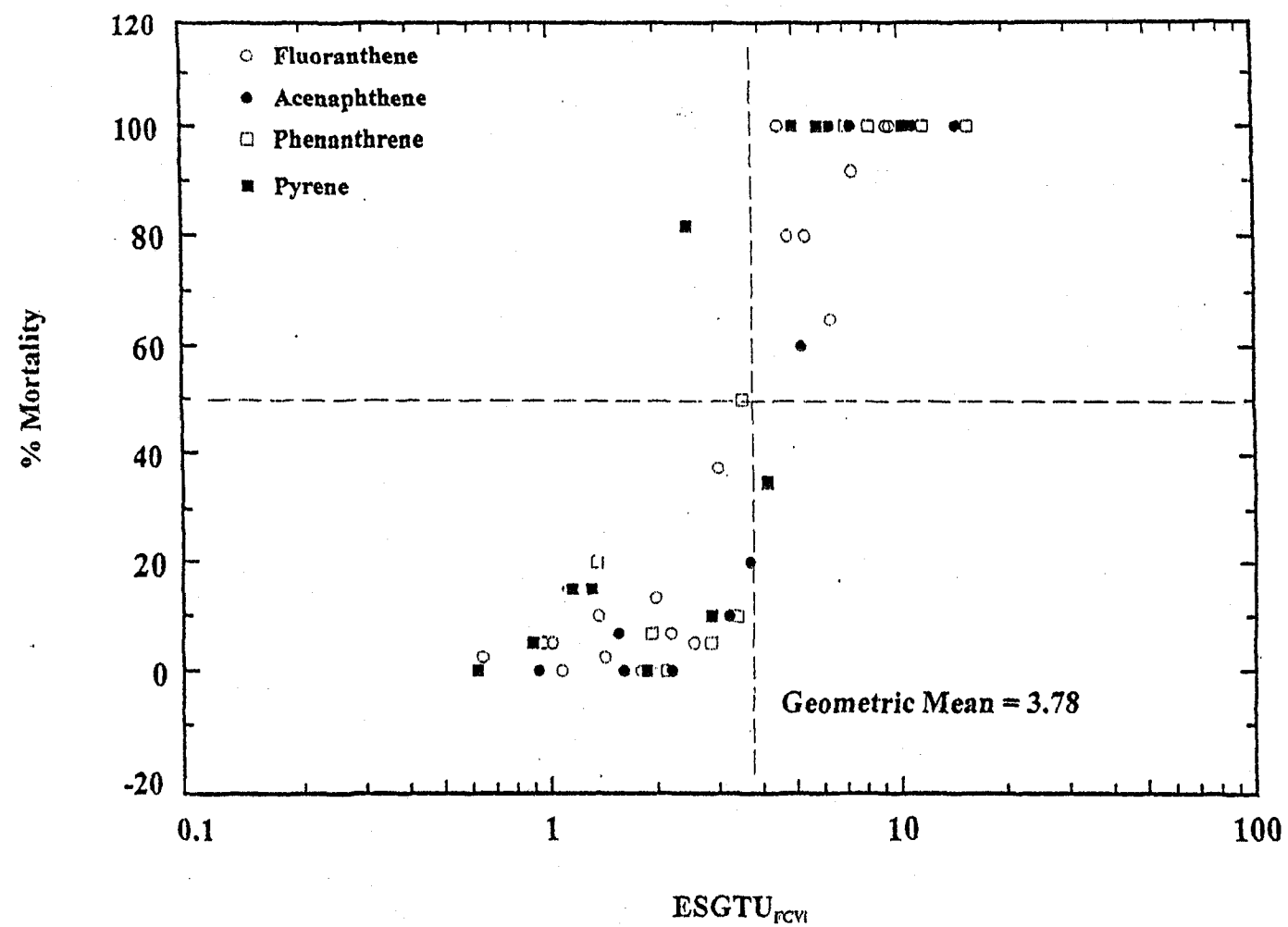
% Less Than or Equal To

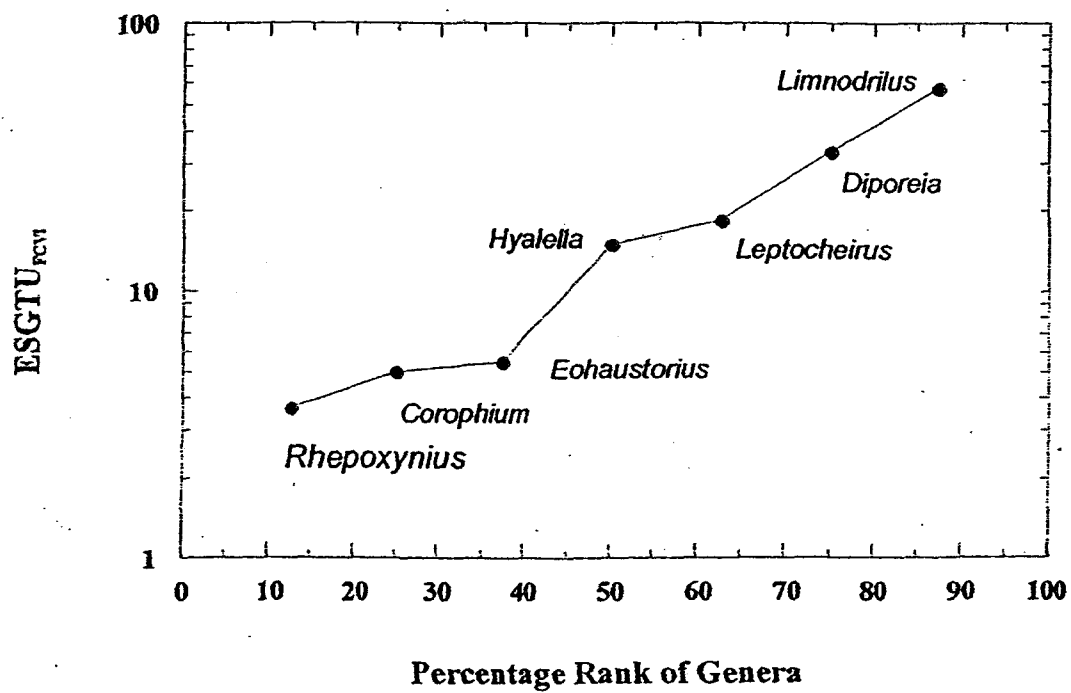
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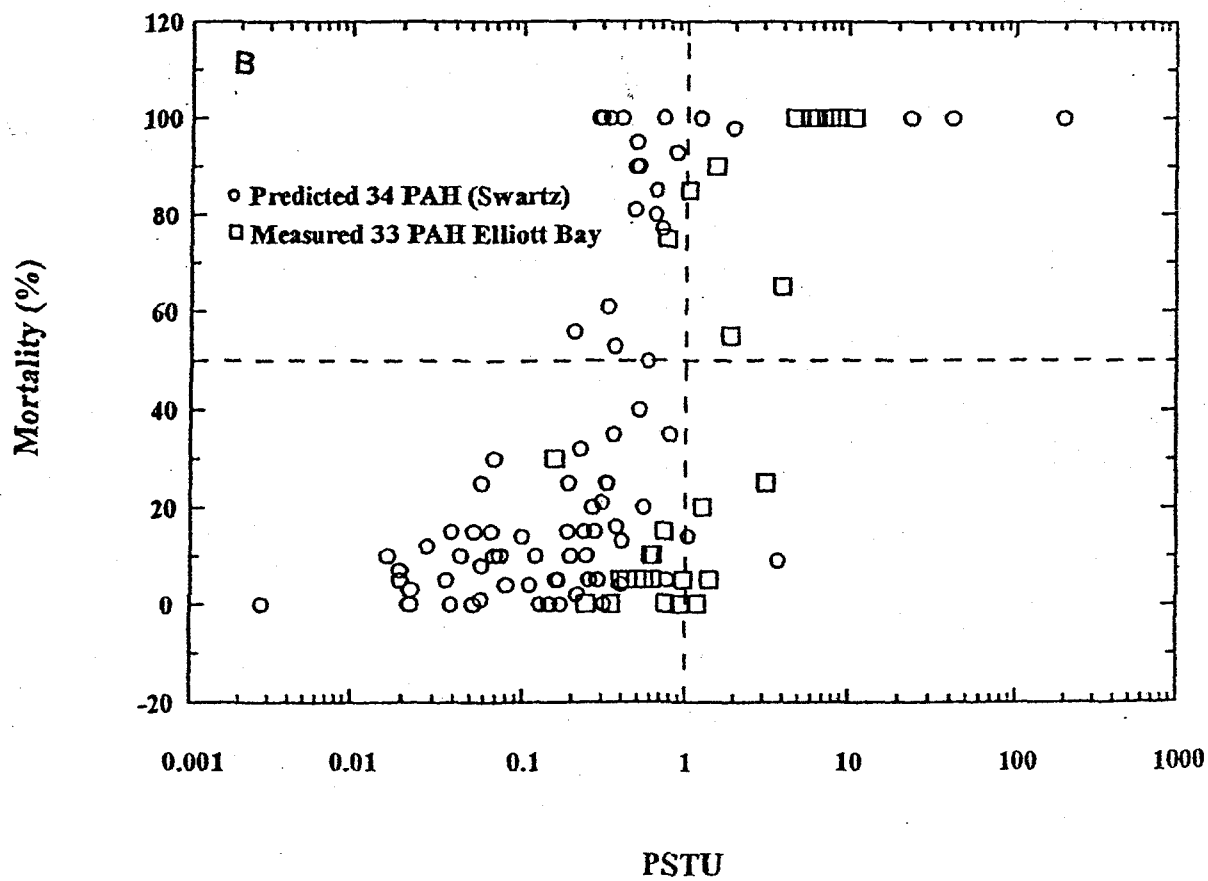
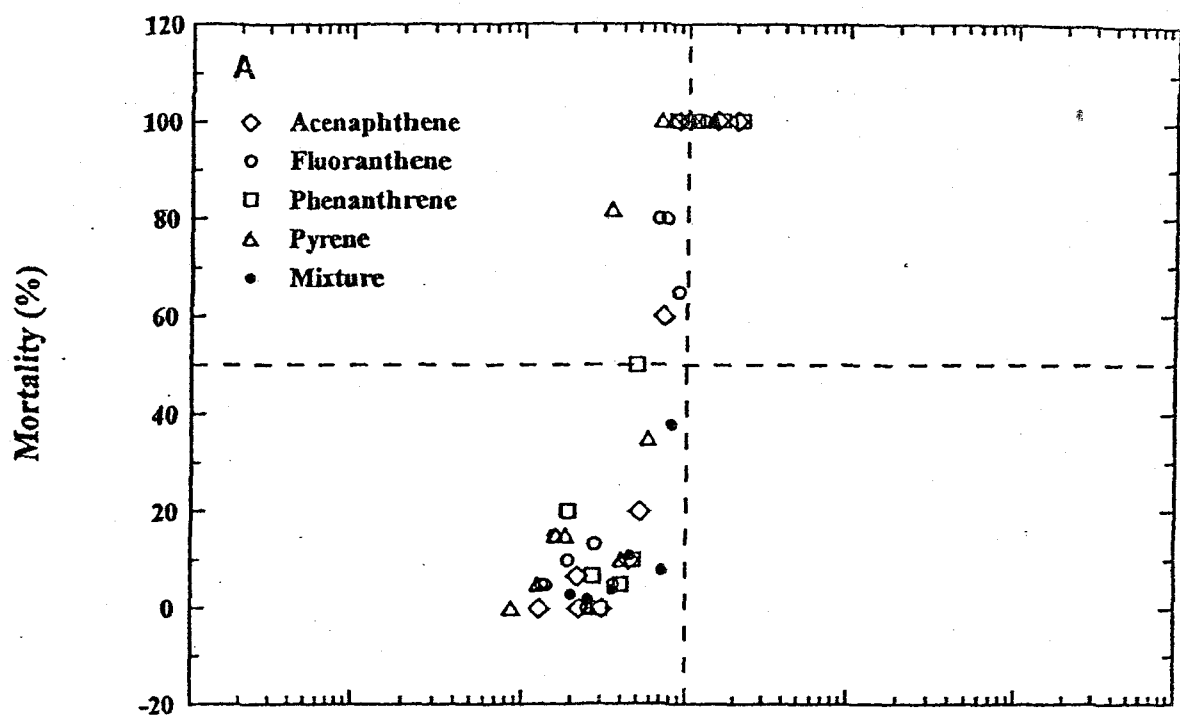


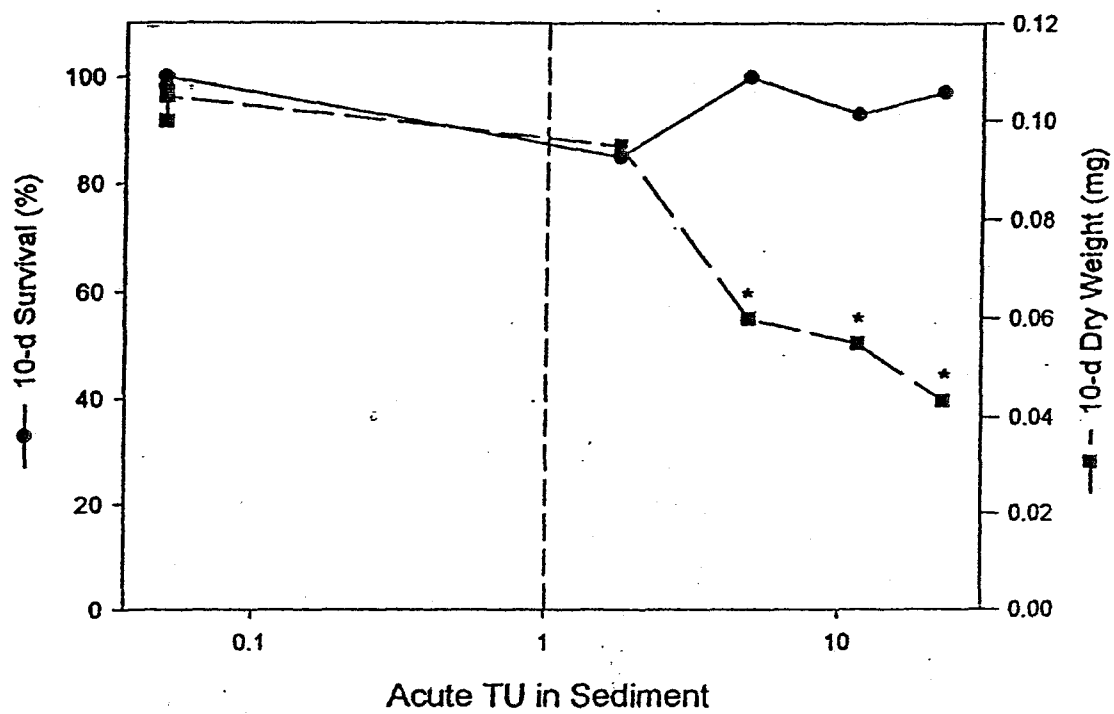


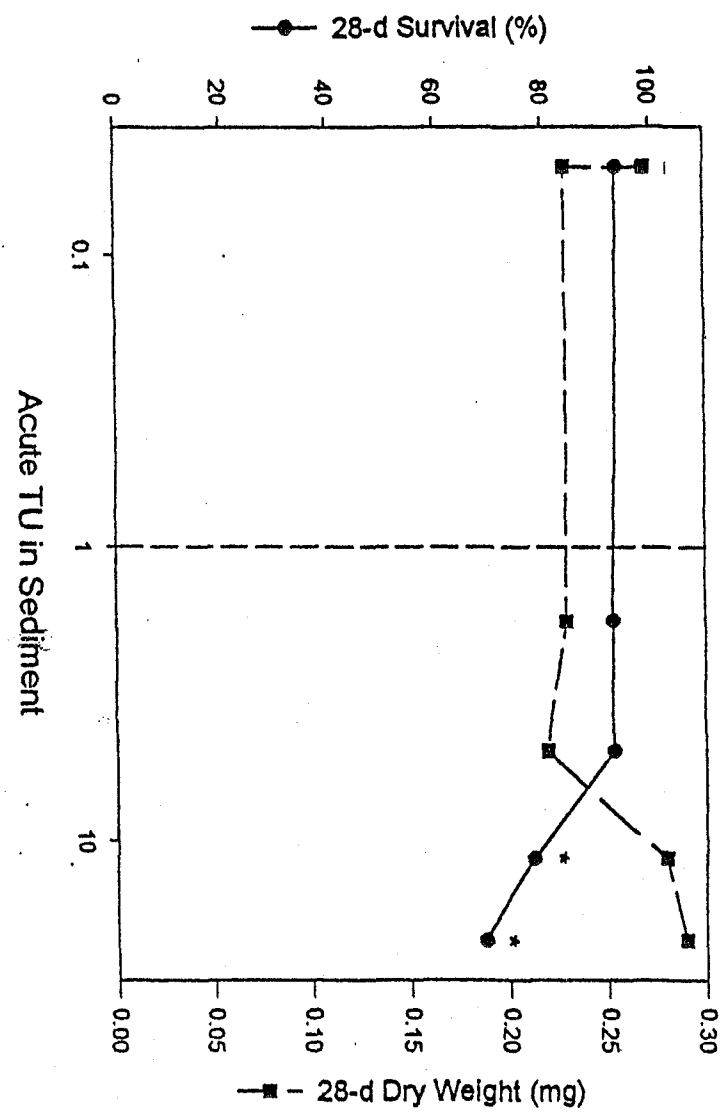


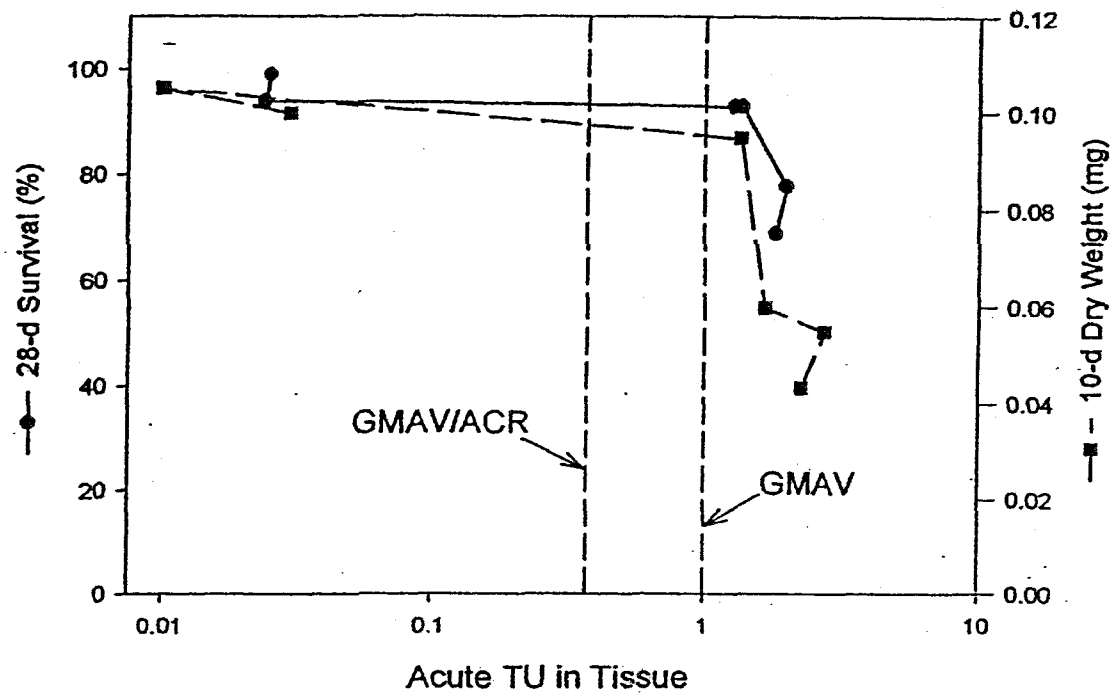


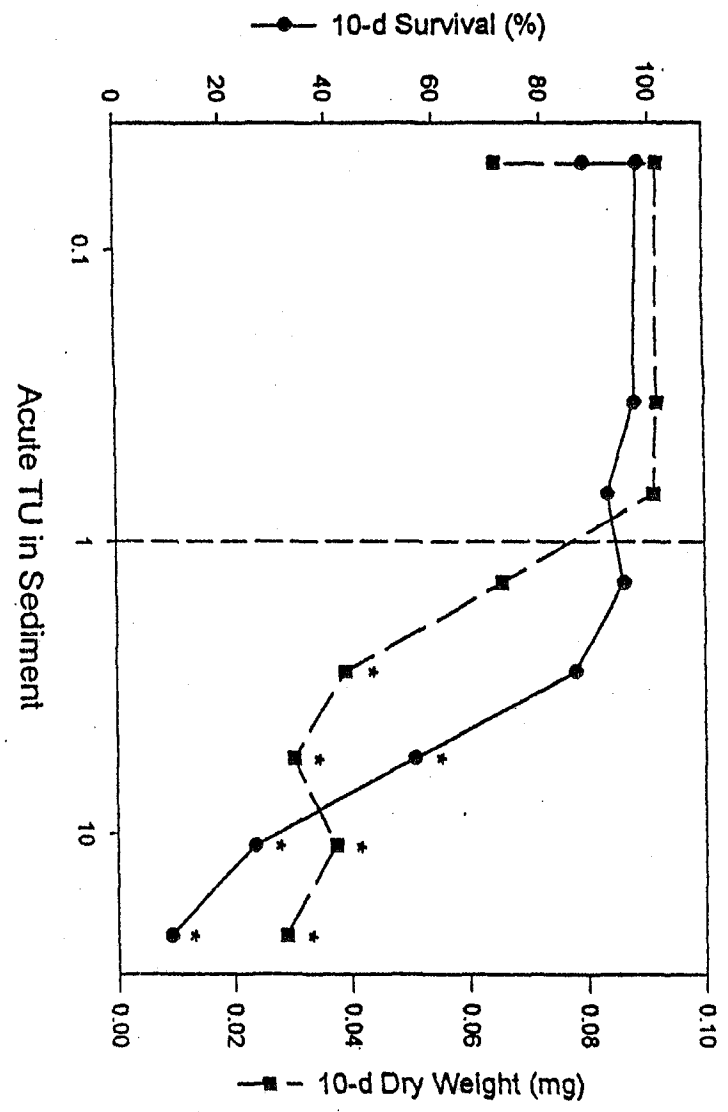


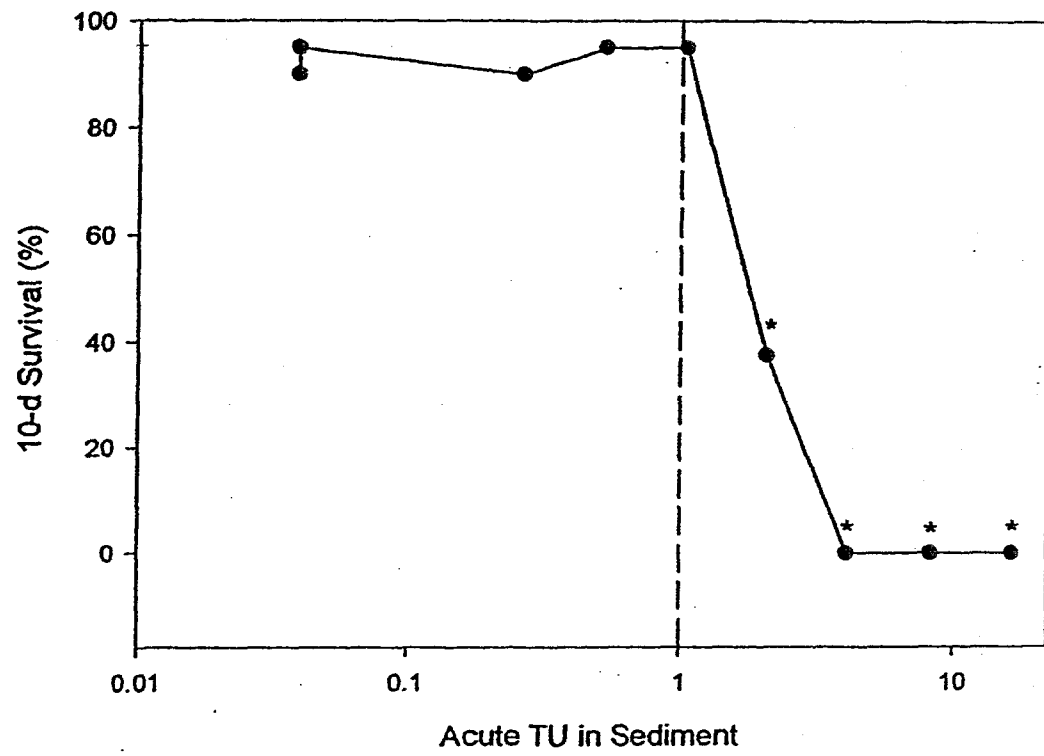


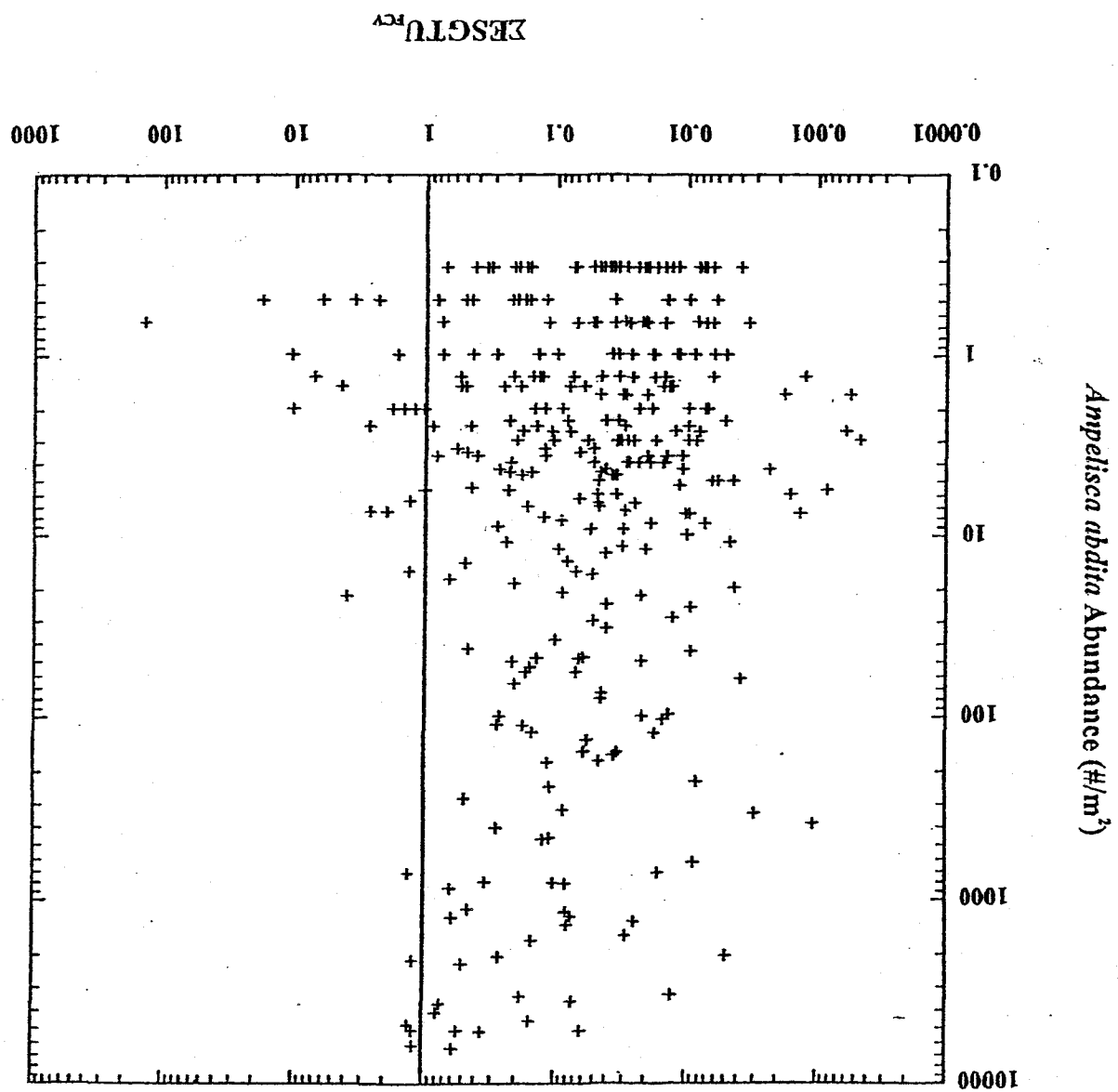


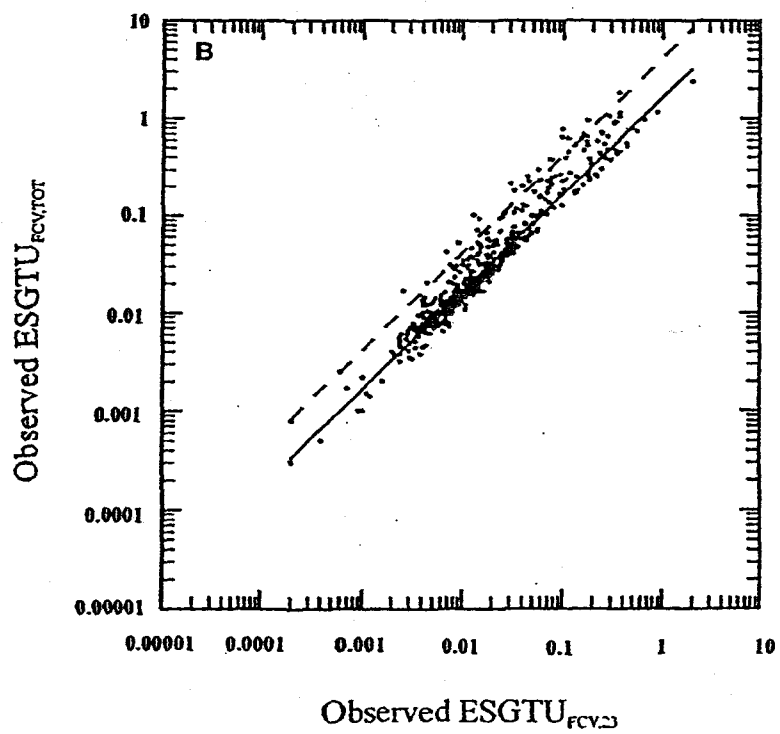
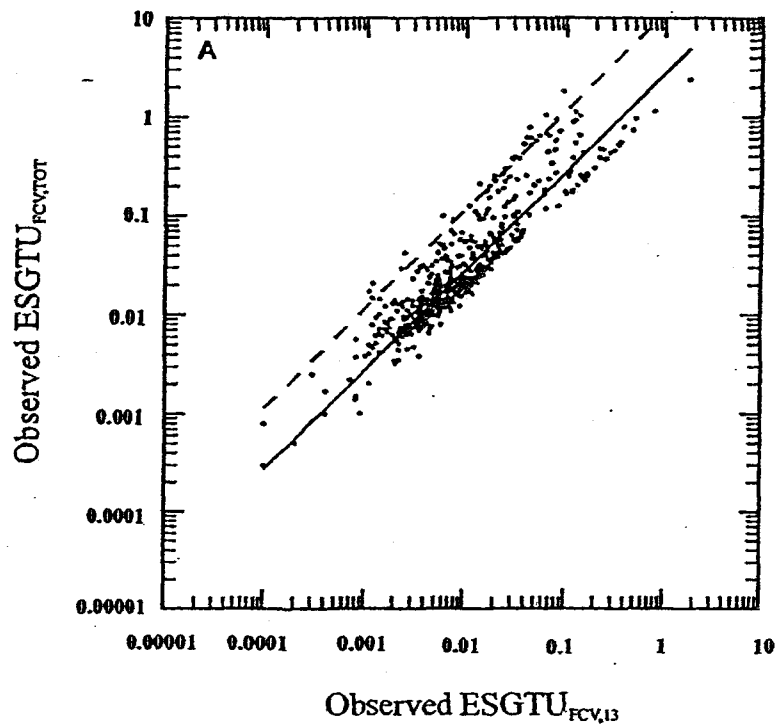


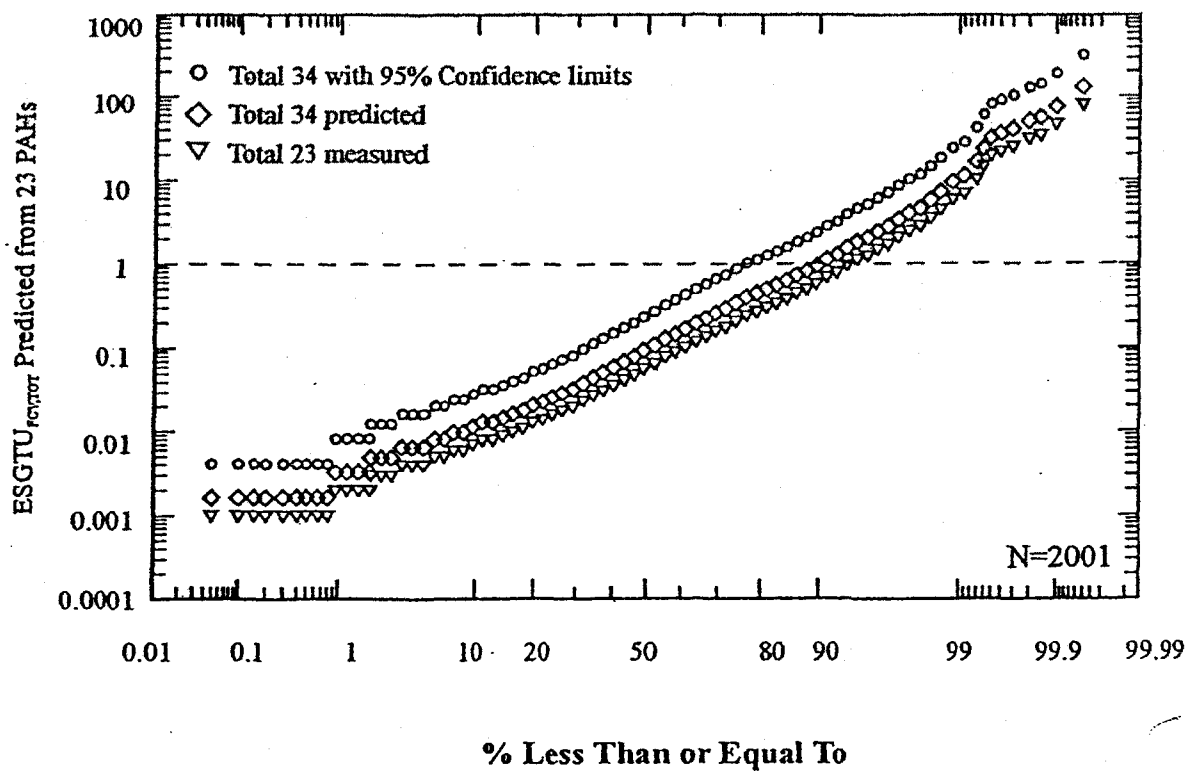
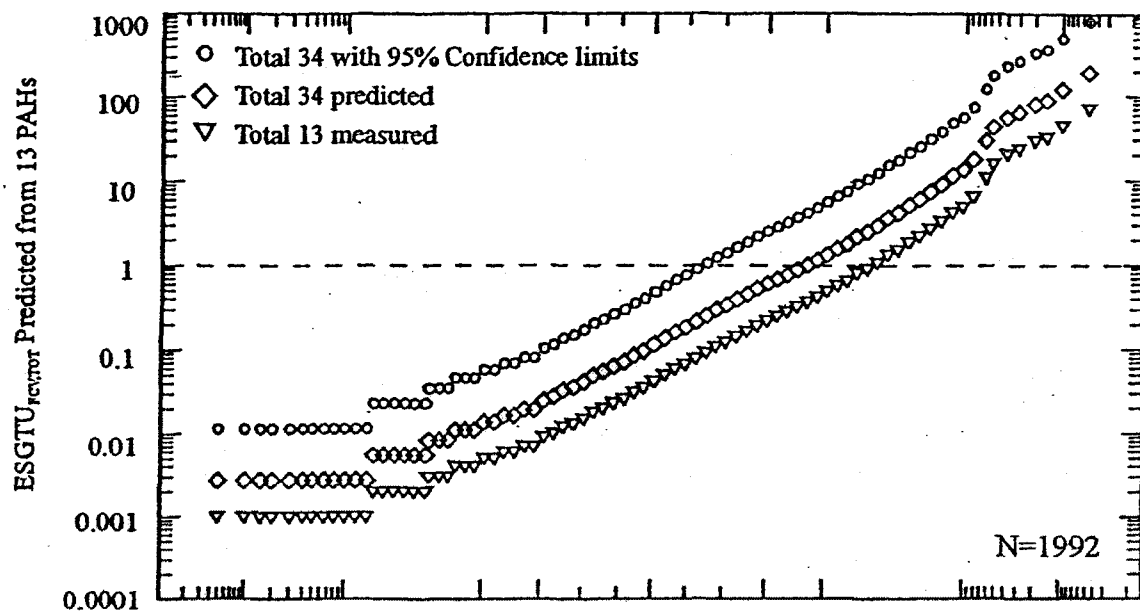


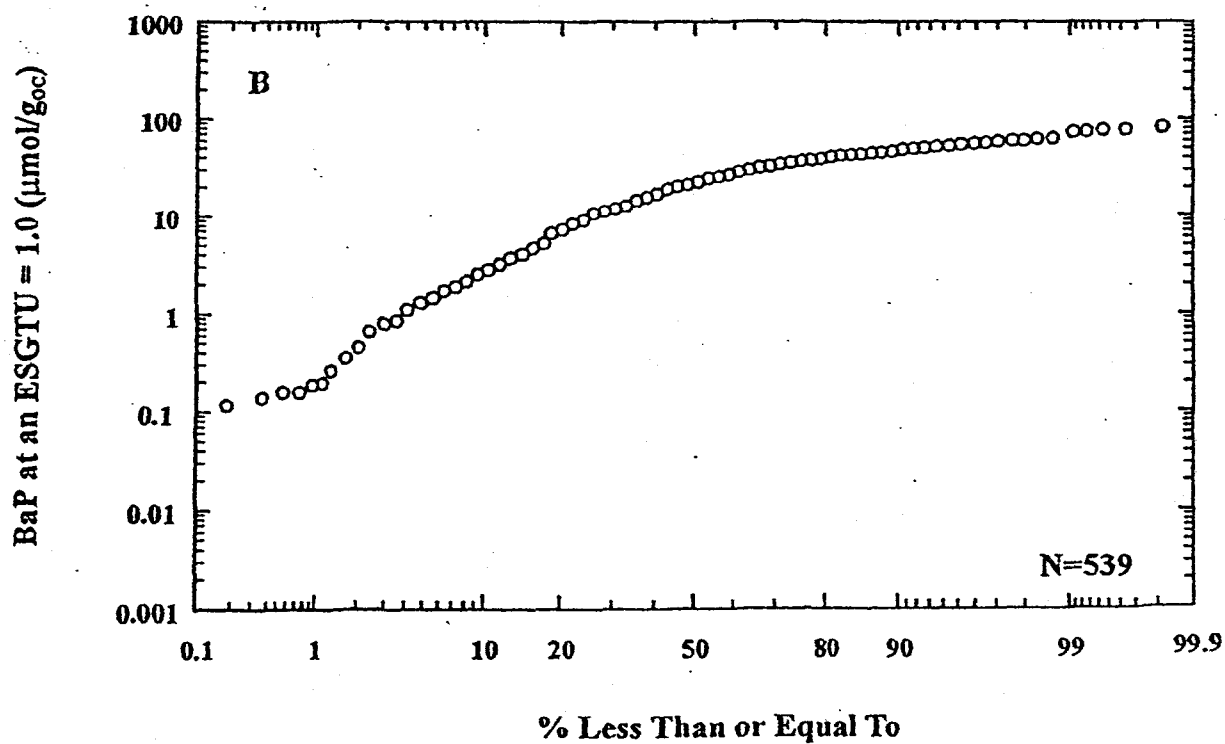
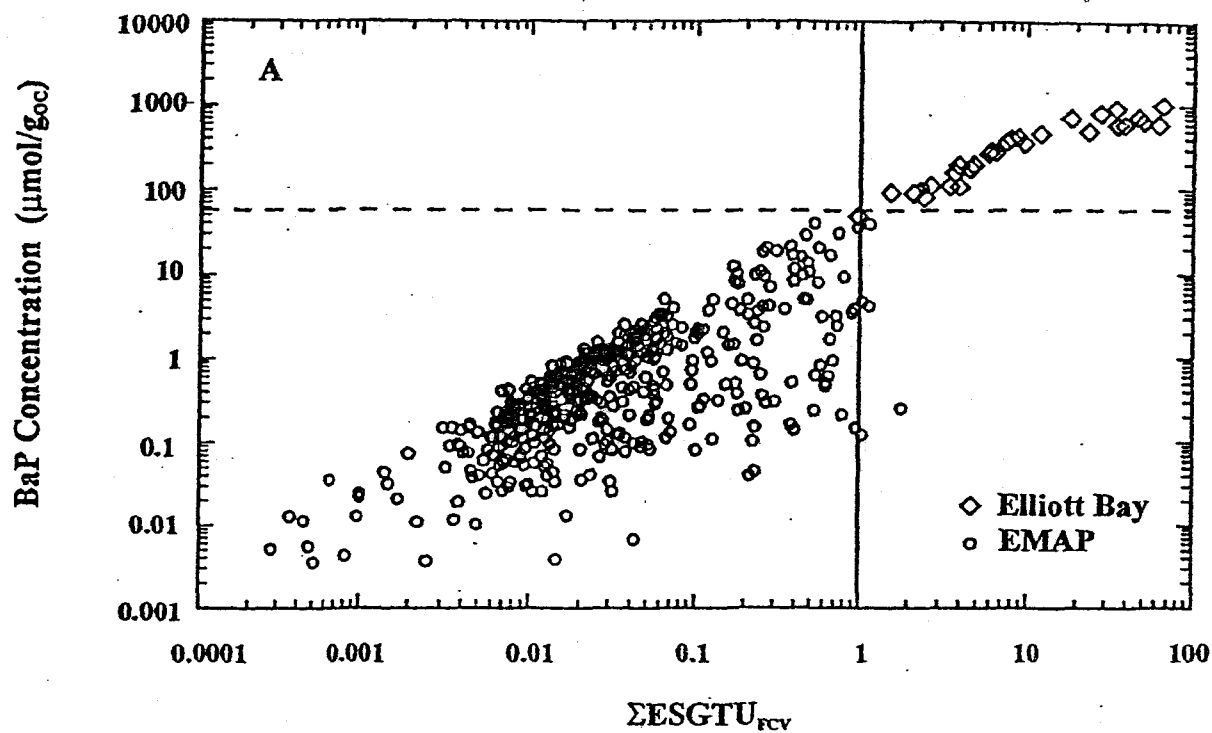




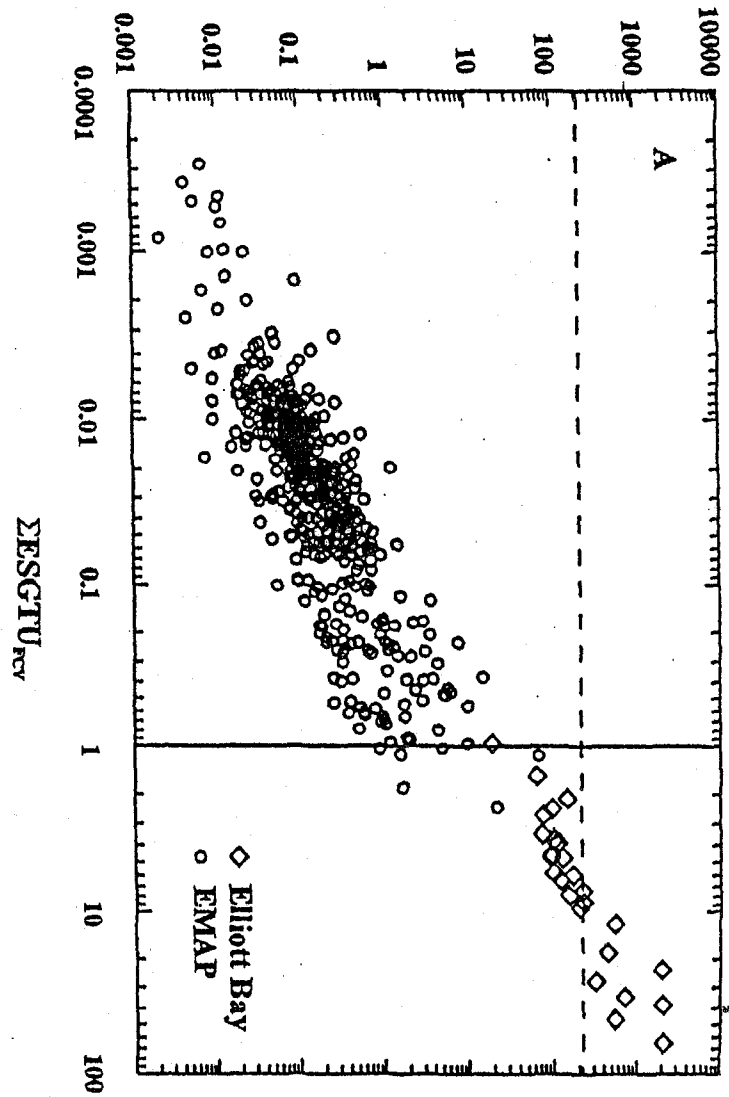




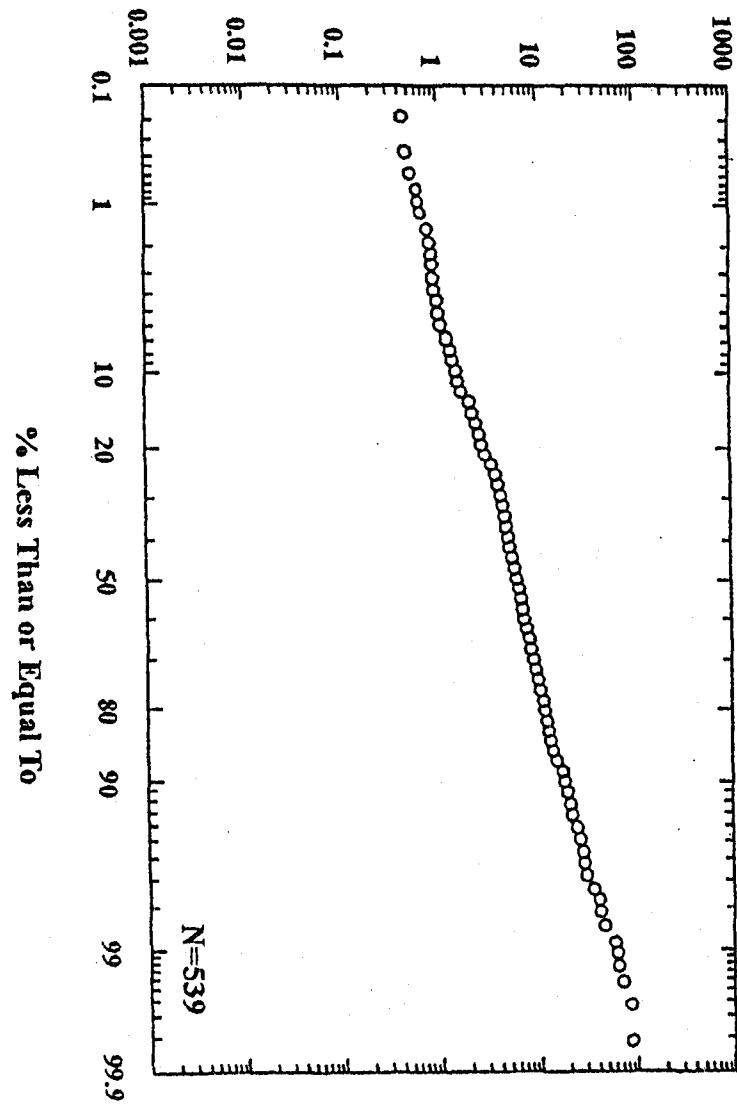




Anthracene Concentration ($\mu\text{mol/g}_{\text{oc}}$)



Anthracene at an ESGTU = 1.0 ($\mu\text{mol/g}_{\text{oc}}$)



Computed concentration divided by concentration at 25

